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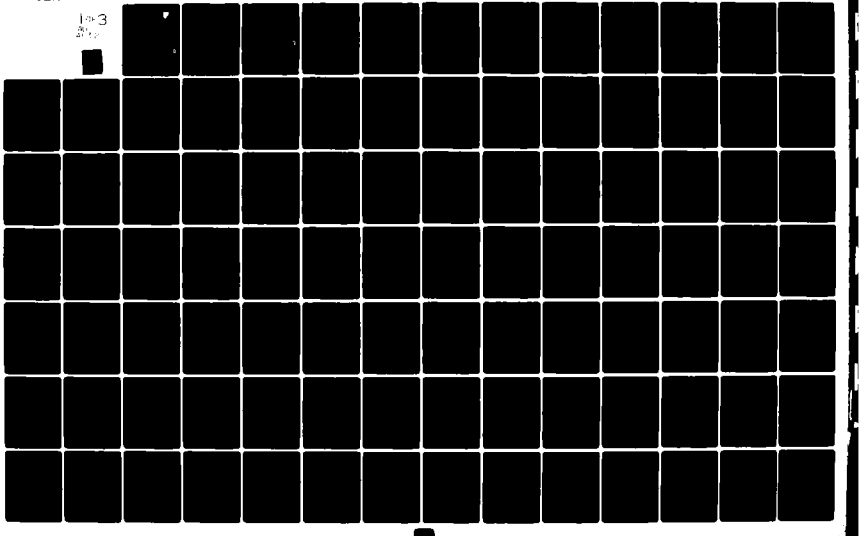

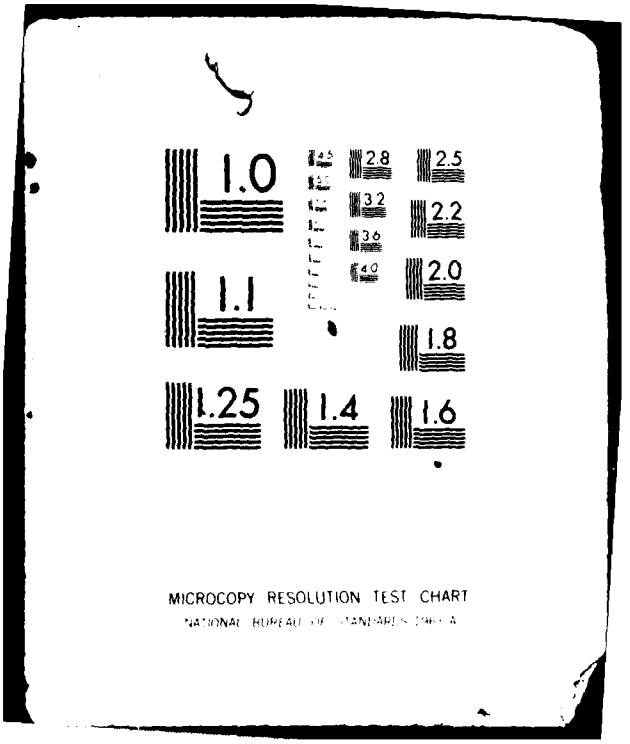
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RADC-TR-82-13
Final Technical Report
February 1982

INVESTIGATION OF THE CURRENT VOLTAGE RELATIONSHIP FOR LOW BARRIER SCHOTTKY DIODES

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A model is developed for the current voltage characteristics of metal, p-type semiconductor Schottky barriers. The model accounts for transition of electrons from the semiconductor valence band to empty states below the metal Fermi energy. These transitions lead to an effective barrier energy that is lower than predicted by classicial models. The model also includes two junction current mechanisms that give rise to higher reverse currents than that predicted classically.

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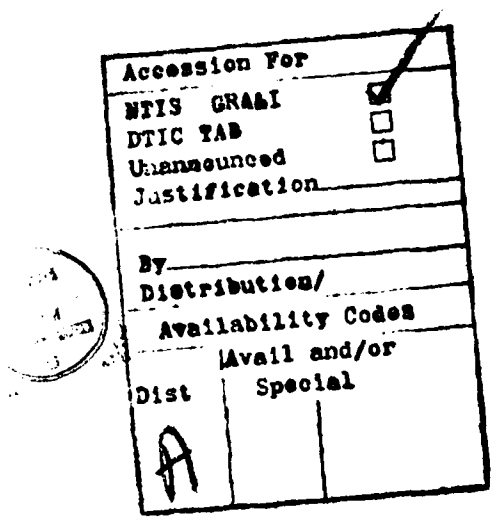
Statement of Work

Under Contract No. 19628-80-C-0020 D.P. Kennedy & Assoc., Inc. has undertaken investigations into the current-voltage relationship of low barrier Schottky diodes. A particular objective of this program was to develop understanding of the large reverse current observed in Pt-Si diodes on p-type silicon, when operating at low temperatures (77° to 110° k). Additionally, after identification of appropriate physical mechanisms it was desired to undertaken rigorous numerical investigations of the topic. Such numerical investigations could offer a means for quantitative comparisons between theory and measurements upon experimental Pt-Si semiconductor devices.



Summary and Major Results

The topic of this investigation was based upon experimental observations of an exceedingly large reverse electric current, as exhibited by p-type Pt-Si Schottky barrier diodes when operating at a low ambient temperature (77° - 110°K). Numerous explanations of this phenomenon are based upon a proposed mechanism of hole generation within metallurgical regions of this device. It has been suggested that such holes transverse the interface barrier, much like conduction electrons in an n-type Schottky barrier diode and, thereafter, produce the observed electric current. Because hole generation, in the classical sense, cannot exist in a metallic conductor, this investigation was directed toward other mechanisms; mechanisms capable of producing a large reverse electric current.

Calculations show that an insignificant number of mobile electrons exist in p-type silicon at low ambient temperatures (77° to 110° K) and, therefore, the observed reverse electric current is unlikely to arise from normal hole/electron pair generation within the silicon space-charge layer. As a consequence, the observed electric current is suggested to arise from mobile hole generation at the silicon-metal interface through mechanisms heretofore given little recognition in the technical literature. Specifically, it is proposed that silicon valence electrons enter unoccupied electron states within the metallic conductor and, thereby, produce mobile holes without a traditional hole-electron pair generation in the semiconductor material.

A study of the technical literature was undertaken on the topic of electron field-emission from silicon. Some experimental data on electron field emission has been interpreted as arising from electron emission from the valence band of p-type silicon. Additionally, using approximation methods other workers have shown that field emission from the valence band should, indeed, be expected from p-type silicon.

It is important to note that these studies of field-emission from silicon were undertaken with no apparent recognition of applicable mechanisms for p-type Schottky barrier diodes.

From traditional theory of metallic conductors, it is shown that a large number of unoccupied energy states exist below the Fermi-level. Additionally, it is shown that interface valence electrons can enter these unoccupied states with a degree of excitation below that required by classical theory for this type of electron transition. As a consequence, an effective energy barrier could be defined for a p-type Schottky barrier that is less than that given by traditional theory of metal-semiconductor contacts.

For a p-type Schottky barrier, detailed calculations are presented for the reverse electric current. These calculations are based upon traditional concepts drawn from the statistical theory of matter. Specifically, the rate is calculated at which electron transitions take place from the semiconductor valence band to the conduction band of the metallic contact. Such calculations have been undertaken for a large assumed range of conduction band free electron density; a range that would include both degenerate semiconductor material and an ideal metal.

Resulting from these calculations is much understanding about the mechanisms involved in the operation of a p-type Schottky barrier. It is demonstrated that despite the experimental observation of bidirectional electric current, a true interface energy barrier exists in only a limited type of p-type semiconductor device. In particular a small reverse electric current can arise from one, or both, of two different mechanisms. A small reverse current can arise from the distribution of unoccupied energy states in the metal conduction band, relative to the energy band structure of the p-type semiconductor material. Additionally, an energy barrier in the classical sense can be shown when the conduction band edge of the metal is at a higher energy than the valence band edge of the semiconductor. This second mechanism will probably exist only if the adjacent

material is a highly degenerate semiconductor, rather than a metal. In line with the basic objectives of this research , many calculations were undertaken on the expected reverse current from low barrier semiconductor devices---defining the interface energy barrier in a manner consistant with current textbook concepts. It is shown that relatively poor rectification characteristics should exist for low barrier devices, if the contacting material is a true metal. If, instead, the contacting material is a degenerate n-type semiconductor the rectification properties could be substantially improved, although in most cases the expected reverse current will be larger than calculated from classical concepts of Schottky barrier operation.

For a rigorous study of this topic a computer program was developed that is capable of calculating the electrostatic potential in a reverse biased Schottky barrier diode, in the presence of a large electric current. This computer program involves the simultaneous solution of Poisson's equation and the mobile hole continuity equation. Two distinctly different hole generation mechanisms are utilized: first, the classical HSR hole-electron generation through a single mid-gap recombination center and, second, hole generation from the top of the valence band. This computer program is capable of accurately calculating the Schottky barrier potential distribution, even in the presence of a large reverse electric current . Insufficient time was available during the present contract period to complete coupling this rigorous solution to the calculation of electron transition at the metal/semiconductor interface.

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Chapter I

Theory of Operation for a p-type Schottky Barrier

1.0 Introduction

Experiment shows that low-barrier Schottky barrier diodes on p-type silicon exhibit poor rectification qualities, even at low ambient temperatures. Such experiments have directed workers toward a rigorous study of physical mechanisms associated with this type of semiconductor device. In particular, the physical mechanisms contributing to a large reverse electric current. Therein we have the basis and direction of the present research on Schottky barrier operation. A principle goal for this research is to undertake a mathematical study of the physics associated with the poor reverse current characteristics of the Schottky barrier diode, placing particular emphasis upon devices composed of Pt-Si on p-type silicon.

An initial survey of the technical literature shows that most theory of Schottky barrier diode operation is based upon devices containing n-type semiconductor material. This theory is in detail and mathematically rigorous. Furthermore, comparisons between theory and experiment are in qualitative agreement, and many are in quantitative agreement, for most of the important characteristics exhibited by this device. A source of difficulty in such comparisons has always been a lack of detailed knowledge about the structure of the metal-semiconductor interface. Theoretical investigations are frequently based upon an idealization of this interface, an idealization that renders the problem tractable from a mathematical and physical point of view.

Nonetheless, it is believed safe to say that an extensive understanding is available on the operation of n-type metal-semiconductor contacts of the rectifying and non-rectifying types. Clearly, because of the similarity between n-type and p-type metal-semiconductor contacts it has been a great temptation to explain p-type device operation using the theory for n-type devices---with, of course, suitable modifications. A particularly difficult extension of this n-type device theory has been the need to explain the reverse current in p-type Schottky barriers, when operating at a low ambient temperature. At low temperatures the hole-electron pair generation is insufficient to explain the large reverse electric current exhibited by this semiconductor diode.

In reverse biased n-type Schottky barrier a nearly unlimited supply of mobile electrons reside within the metallic contact. If, indeed, within this source some electrons have sufficient energy to overcome the interface potential barrier, these electrons will contribute to the reverse electric current. Contrasting with this n-type device concept, no such obvious supply of moble carriers exists for the p-type Schottky barrier. It is evident that the reverse electric current in a p-type device arises from holes moving from the depletion layer to charge neutral regions of the semiconductor. An important question is the source of these holes, particularly at an ambient temperature that decreases generation/recombination to a negligible value.

It has been a generally accepted practice to assume hole generation within the metallic contact of a p-type Schottky barrier and, thereby, imply a substantial degree of similarity between n-type and p-type device operation. If, indeed, holes were generated in the metal, the theory of p-type diode operation would be a simple extension of n-type device theory. It must be acknowledged that mobile holes, as such, cannot exist within a metallic conductor and, therefore, the theory of p-type Schottky barrier operation is in great difficulty.

There is little question that the reverse electric current must arise from mobile holes within the space-charge region of a p-type device. Additionally, it must be acknowledged that these mobile holes do not arise from hole-electron pair generation alone. If generation/recombination mechanisms represented the only source of mobile holes, we could not explain the large magnitude of reverse current at low device temperatures. Instead, new mechanisms of hole generation must be proposed; mechanisms whereby mobile holes are generated without necessarily generating conduction band electrons.

The basis of the present research is to investigate a new mechanism of the foregoing type. Specifically, it is proposed that hole generation can exist at the metal-semiconductor interface by valence electron transitions from the semiconductor to unoccupied states within the metallic conductor. Further, it is suggested that through this mechanism we can explain the low temperature reverse electric current characteristics exhibited by low-barrier Schottky devices on p-type silicon. Additionally it is suggested that this mechanism will often render such a physical structure electrically Ohmic at room temperature.

2.0 Field Emission from Semiconductor Materials

For many years electron emission from electrical conductors has been a topic of extensive investigation. There are two basic mechanisms whereby this emission can take place: first, at high temperatures (Thermionic emission) and, second, when a conductor is exposed to a large electric field in a direction normal to its surface (Field emission). At high temperatures free electrons within a conductor acquire sufficient energy to overcome an electrostatic potential barrier present at its surface. At large values of normally directed electric field the surface barrier of a material can become exceedingly thin and, thereby, permit tunneling from the material to free space.

Emission experiments using semiconducting material have brought renewed interest to this subject. In particular, two distinctly different field-emission characteristics can be demonstrated for n-type and p-type silicon and germanium [1-4]. Further, some experiments show that n-type silicon can exhibit the field emission properties of n-type or p-type silicon. These two distinctly different emission characteristics have been explained theoretically [5] ; the first type is proposed to result from the emission of valence band electrons.

It is emphasized that these studies were directed toward the topic of field-emission, with no reference to implications associated with device theory. Nonetheless, field-emission from the valence band represents hole generation without the generation of an associated conduction band electron. If, indeed, these field-emission workers demonstrate valence band emission from silicon, there is little reason to neglect this mechanism in the theory of Schottky barrier diode operation.

3.0 Unoccupied Energy States in a Metallic Conductor

In the present discussion we focus upon the density and distribution of unoccupied energy states in a conductor that reside between the Fermi-level E_f and the conduction band edge E_c. It will be shown that a significant quantity of these unoccupied states are far removed from the Fermi-level, and there is no reason to assume $E_f - E_b$ in Fig.1 represents a real energy barrier in a p-type Schottky device. In particular many silicon valence electrons at the metal-semiconductor interface that undergo thermal excitation can, indeed , enter the metal at an energy substantially below the traditionally assumed Fermi-level.

The distribution of unoccupied energy states is particularly dependent upon the position of the Fermi-level, relative to the conduction band edge. Additionally, this Fermi-level is temperature dependent; we must first establish its magnitude, as a function of temperature. This

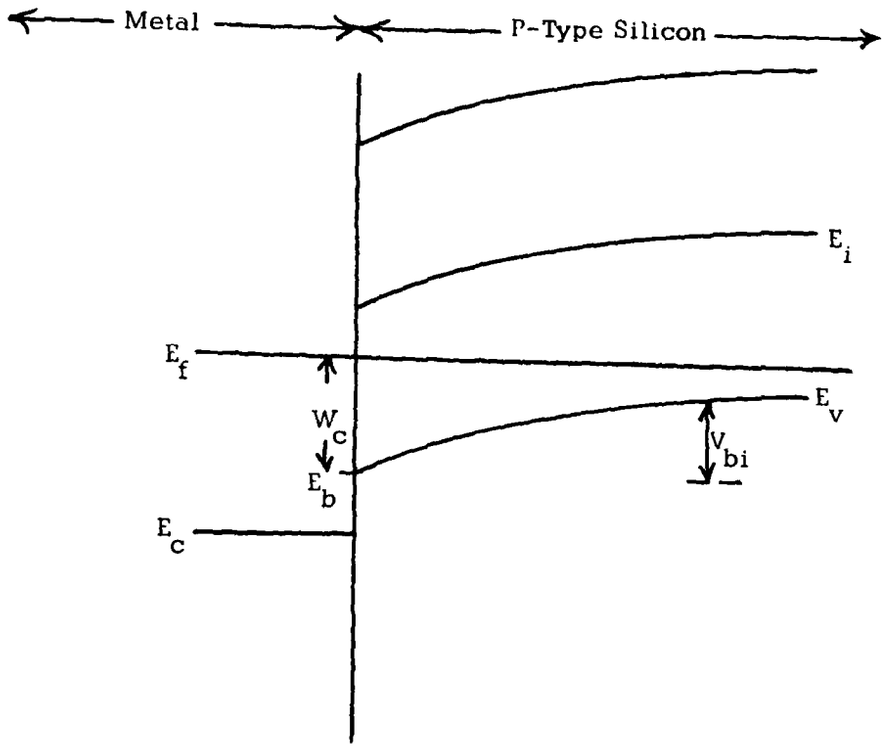

Fig.1 Energy Band Diagram for a Schottky Barrier on P-Type Silicon

is easily accomplished using the conventional density of states equation [6],

$$\Delta N = 8\pi\sqrt{2}\,(\sqrt{m}/h)^3\sqrt{E}\;\Delta E \tag{1-1}$$

in combination with the Fermi-Dirac distribution

$$P(E) = \left[1 + \exp\,(E - E_f) / kT\right]^{-1} . \tag{1-2}$$

Upon combining Eq.(1-1) and Eq.(1-2) we have the familiar density of occupied energy states that reside between E and (E + ΔE),

$$\Delta N = 8\pi\sqrt{2}\,(\sqrt{m}/h)^3\sqrt{E}\left[1 + \exp\,(E - E_f) / kT\right]^{-1}\Delta E \tag{1-3}$$

clearly, the total density of these occupied states in a metal is given by

$$N_c = 8\pi\sqrt{2}\,(\sqrt{m}/h)^3 \int_0^\infty \frac{\sqrt{E}\;dE}{1 + \exp\,(E - E_f) / kT} \tag{1-4}$$

Equation (1-4) has been used to calculate the Fermi-level in a metal as a function of temperature. We first assume in Eq.(1-4) that T = 0 yielding

$$N_c = 8\pi\sqrt{2}\,(\sqrt{m}/h)^3\left[\frac{2}{3}\;E_{f0}^{3/2}\right] \tag{1-5}$$

where N_c is the density of conduction electrons and E_{f0} is the Fermi energy at T = 0. Thereafter, we combine Eq.(1-4) and Eq.(1-5) and solve for E_f

$$1 = \frac{3}{2} \; E_{f0}^{-3/2} \int_{0}^{\infty} \frac{\sqrt{E}\; dE}{1 + \exp\,(E - E_f) / kT} \; . \qquad (1\text{-}6)$$

Figure 2 illustrates this Fermi-level calculation assuming a density of states effective mass of unity. Clearly, calculating the Fermi-level is an iterative process and must be accomplished through numerical integration techniques; the computer program used for this calculation is listed in APPENDIX IA. In all calculations presented in this report the foremention computer program was used for calculating the Fermi-level.

Only a minor modification of Eq.(1-4) is required to calculate the density of unoccupied energy states that reside between the Fermi-level and the conduction band edge,

$$N = 8\pi \sqrt{2} \; (\sqrt{m} / h)^3 \int_{Ec}^{E_f} \frac{\sqrt{E}\; dE}{1 + \exp\,(E - E_f) / kT} \; . \qquad (1\text{-}7)$$

Figure 3 illustrates this calculation throughout a wide temperature range, and throughout a range of free electron density frequently encountered in a metallic conductor.

From Fig.3, at 77° K conductors with a free electron density within the range $10^{20} \leq Nc \leq 10^{23}$ can be expected to contain about 10^{18} to 10^{19} unoccupied energy states between the Fermi-level and the conduction band edge. Clearly, this is a non-negligible quantity if we wish to assume $E_f - E_b$ in Fig.1 represents an energy barrier that limits the reverse electric current in a Schottky diode.

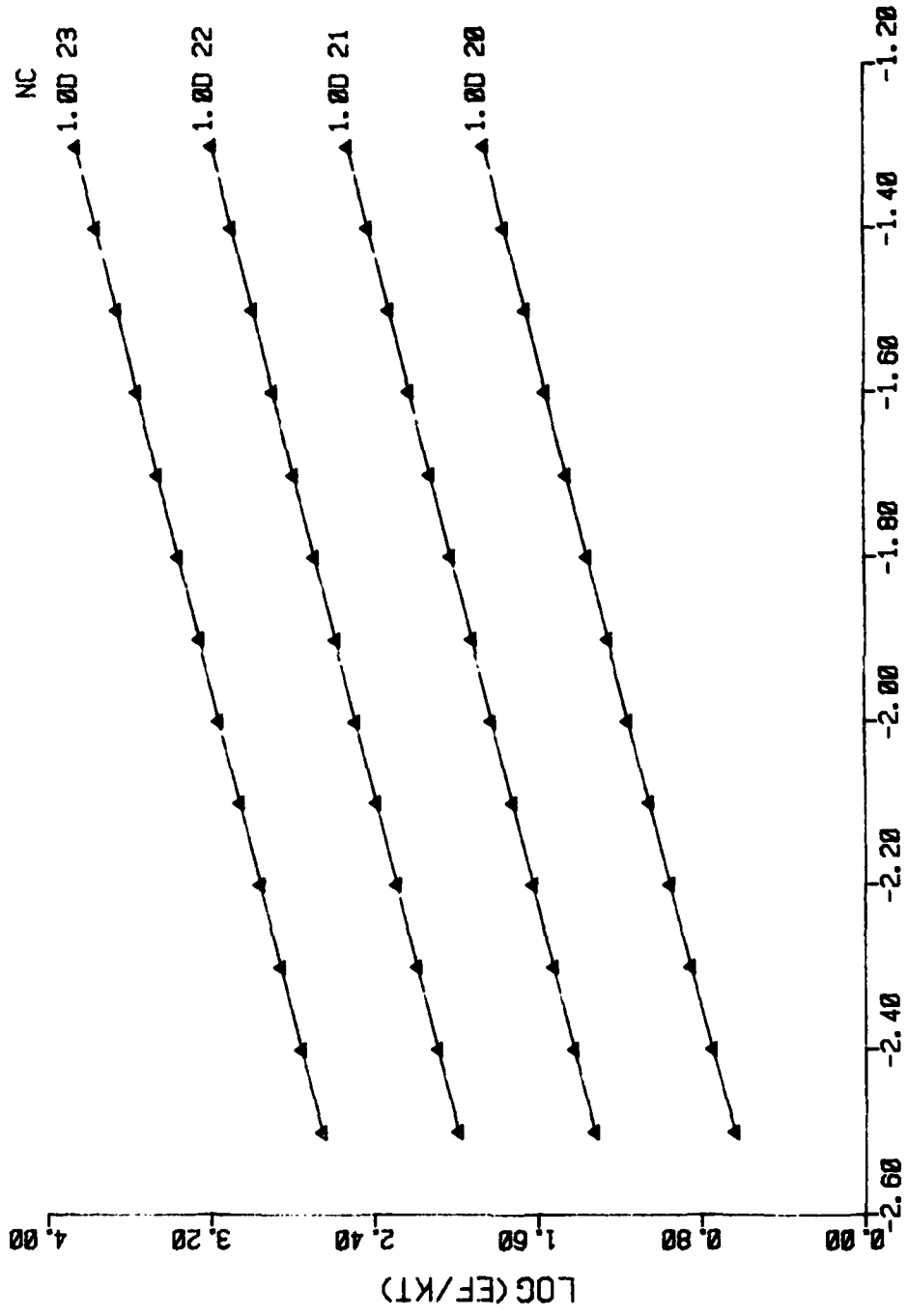

Fig.2 Fermi Level in a Metal Containing a Free Electron Density of N_c

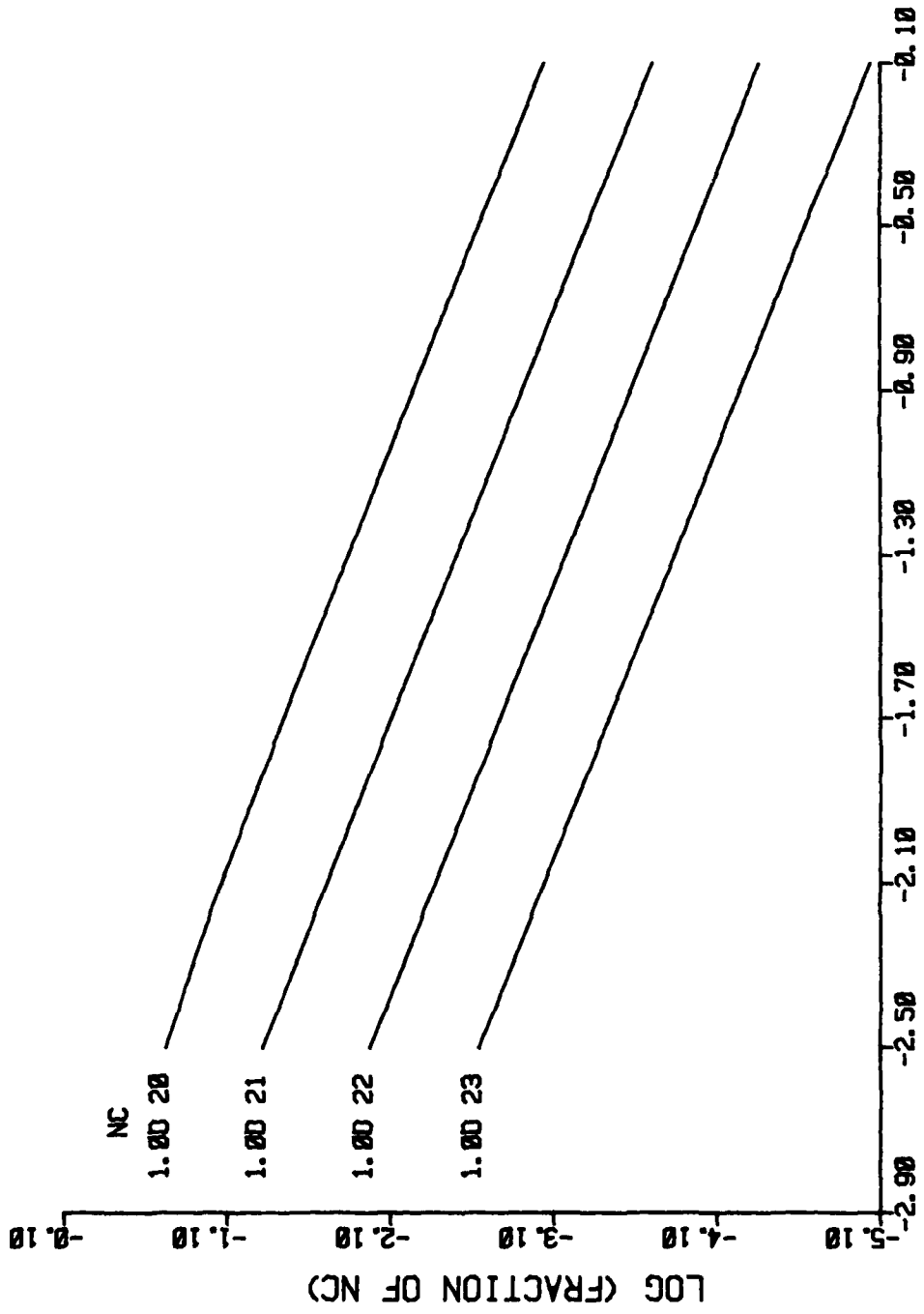

Fig.3 Density of Unoccupied Energy States in a Metal Between the Conduction Band Edge E_c and the Fermi-Level. N_c = Free Electron Density

An equally important aspect of this concept is the distribution of these unoccupied energy states within the range $E_c \prec E \prec E_f$. Clearly, if the majority of these unoccupied states are clustered near the Fermi-level we could retain the concept of a potential barrier of $E_f - E_b$ in a Schottky diode. If, instead, a large quantity of states reside near the energy E_b in Fig.1, we must reconsider the concept of reverse electric current in this semiconductor device.

Again, by numerically integrating the expression

$$N = 8\pi\sqrt{2}\,(\sqrt{m}/h)^3 \int_{E_b}^{E_f} \frac{\sqrt{E}}{1 + \exp(E - E_f)/kT} \qquad (1\text{-}8)$$

We evaluate the quantity of unoccupied states that reside throughout the energy range $E_b \leq E \leq E_f$. Such calculations are presented in Fig. 4 through Fig. 6 for a range of assumed locations for E_b.

This sequence of calculations clearly show that the density of unoccupied states are, indeed, clustered near the Fermi-level. For example, material containing a free electron density of 10^{22} (cm^{-3}), Fig.(6), exhibit a negligible difference in vacant state density between $E_b/E_f = 0.1$ and $E_b/E_f = 0.98$, at a temperature of 77° K. Similarly, at room temperature material with a free electron density of 10^{21} (cm^{-3}), Fig.5, exhibits an unoccupied energy state density of about 1.25×10^{19} (cm^{-3}) within 2% of the range ($E_f - E_b$) from the Fermi-level. Nonetheless, it is recognized that in a Schottky diode the remaining unoccupied energy states could produce a significant magnitude of reverse current.

A further amplification of this topic is obtained by numerically integrating Eq.(1-4) throughout the range $E_c \leq E \leq E_b$,

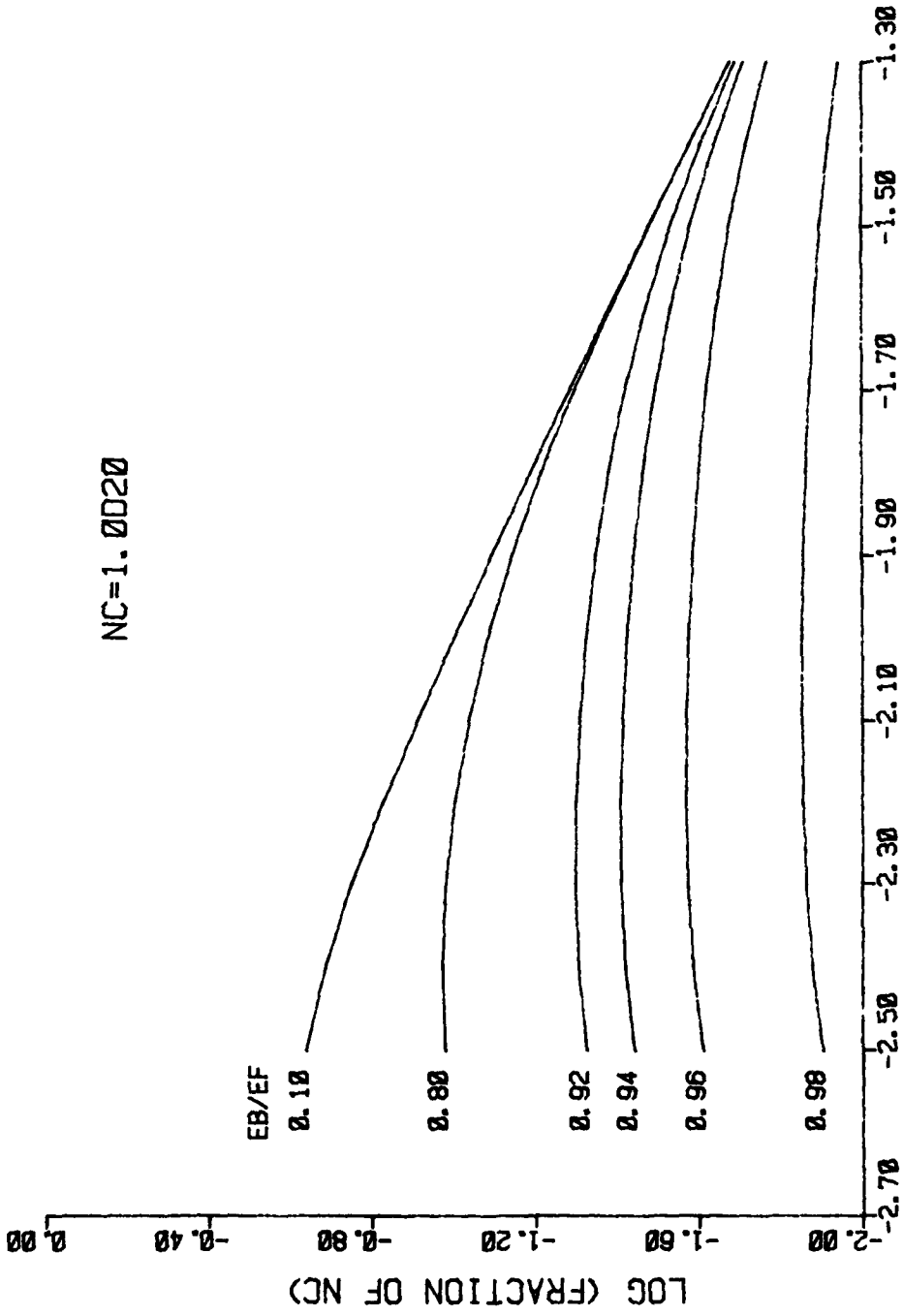

Fig.4 Density of Unoccupied Energy States Between the Fermi-Level, E_f and an Energy E_b where $E_c < E_b < E_f$

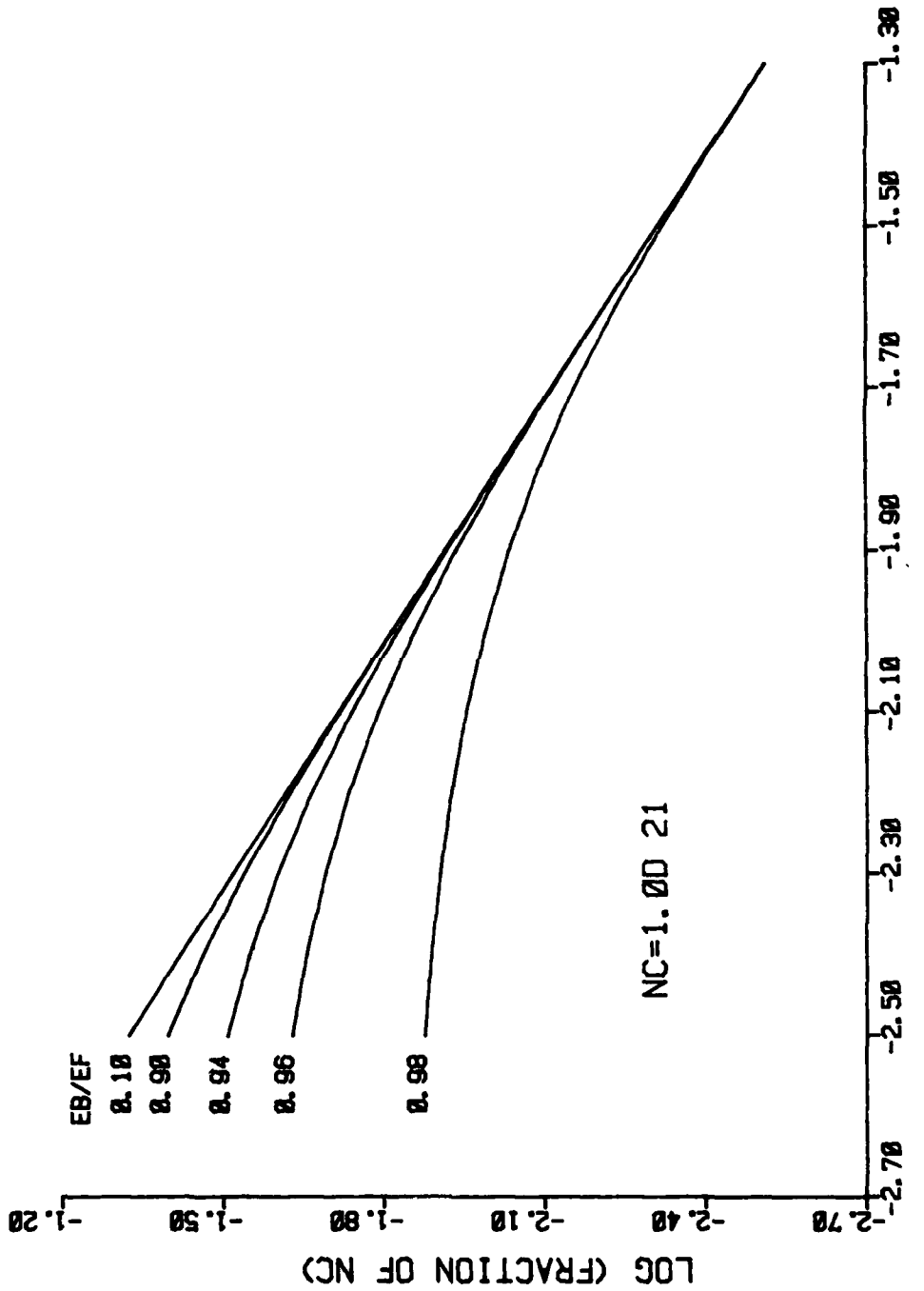

Fig.5 Density of Unoccupied Energy States Between the Fermi-Level and an Energy E_b where $E_c < E_b < E_f$

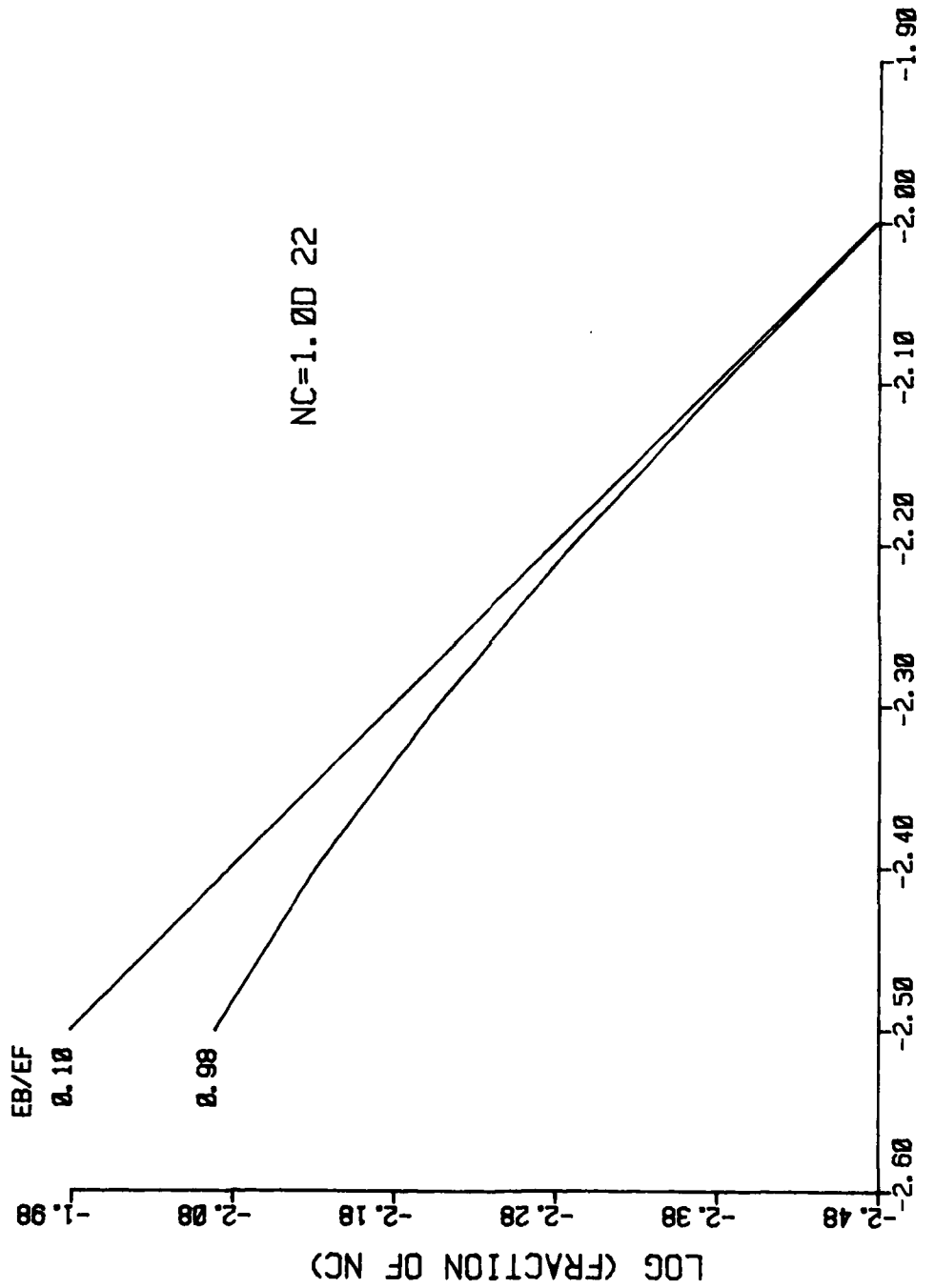

Fig.6 Density of Unoccupied Energy States Between the Fermi Level E_f and an Energy E_b where $E_C < E_b < E_f$

$$N = 8\pi\sqrt{2}\,(\sqrt{m}/h)^3 \int_{E_c}^{E_b} \frac{\sqrt{E}\;dE}{1 + \exp(E_f - E_c)/kT} \quad . \qquad (1\text{-}9)$$

This calculation yields the density of unoccupied states that reside in the lower energy regions of the conduction band.

Figure 7 through Fig.10 illustrate this calculation throughout a range of free electron density of $10^{20} \leq Nc \leq 10^{23}$. These calculations clearly show that material containing a larger free electron density have the smallest density of unoccupied states in the lower regions of the conduction band. For example, at 77° K a free electron density of 10^{20} (cm^{-3}), Fig.7, exhibits about 10^{14} (cm^{-3}) unoccupied states in the lower 50% between E_f and E_c. At this same temperature material containing a free electron density of 10^{22} (cm^{-3}) contain approximately 10^{8} (cm^{-3}) unoccupied states in the lower 92% of the energy between E_f and E_c.

The reason for this foregoing situation is attributable to the increase of $(E_f - E_c)$ with free electron density, Fig.2. An increase of $E_f - E_c$ produces a decrease of probability that the lower energy electrons can be excited to an energy level above E_f.

In the following sections of this report the computer programs used for calculations thus far illustrated are an integral part of all calculations directed toward the operation of Schottky barrier devices.

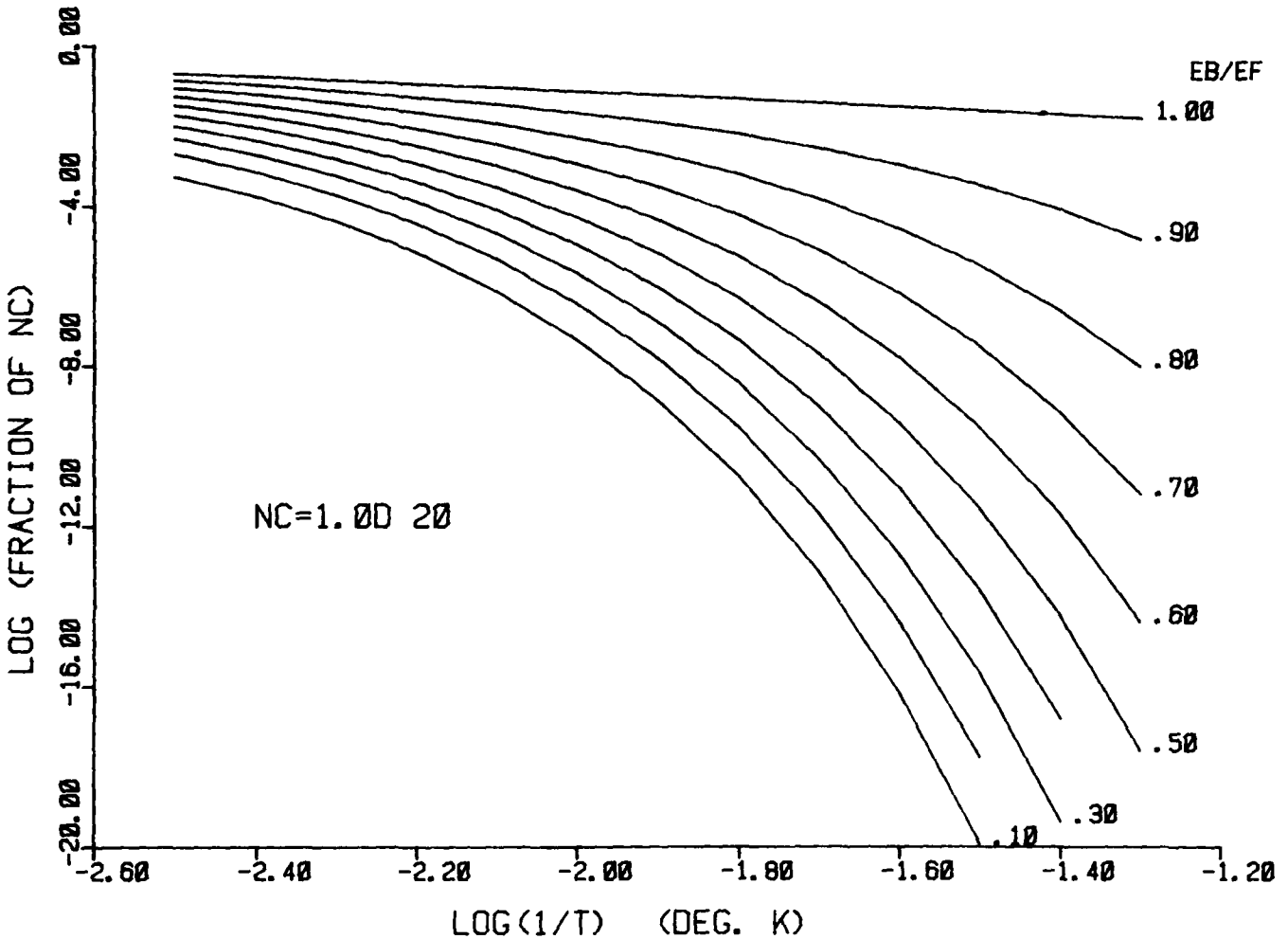

Fig.7 Density of Unoccupied Energy States Between the Conduction Band Edge E_c and an Energy E_b where $E_c < E_b < E_f$

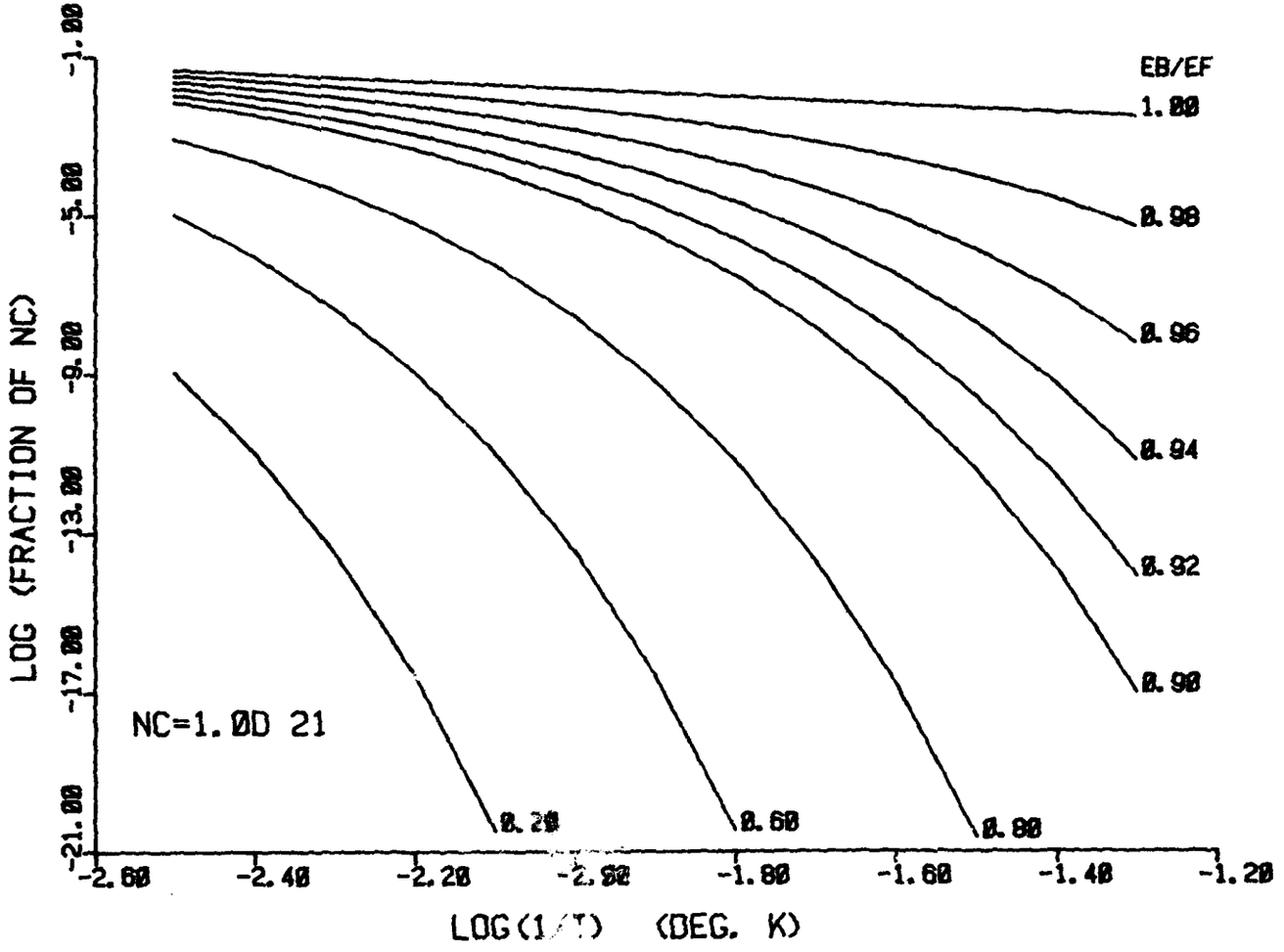

Fig. 8 Density of Unoccupied Energy States Between the Conduction Band Edge and an Energy E_b where $E_c < E_b < E_f$

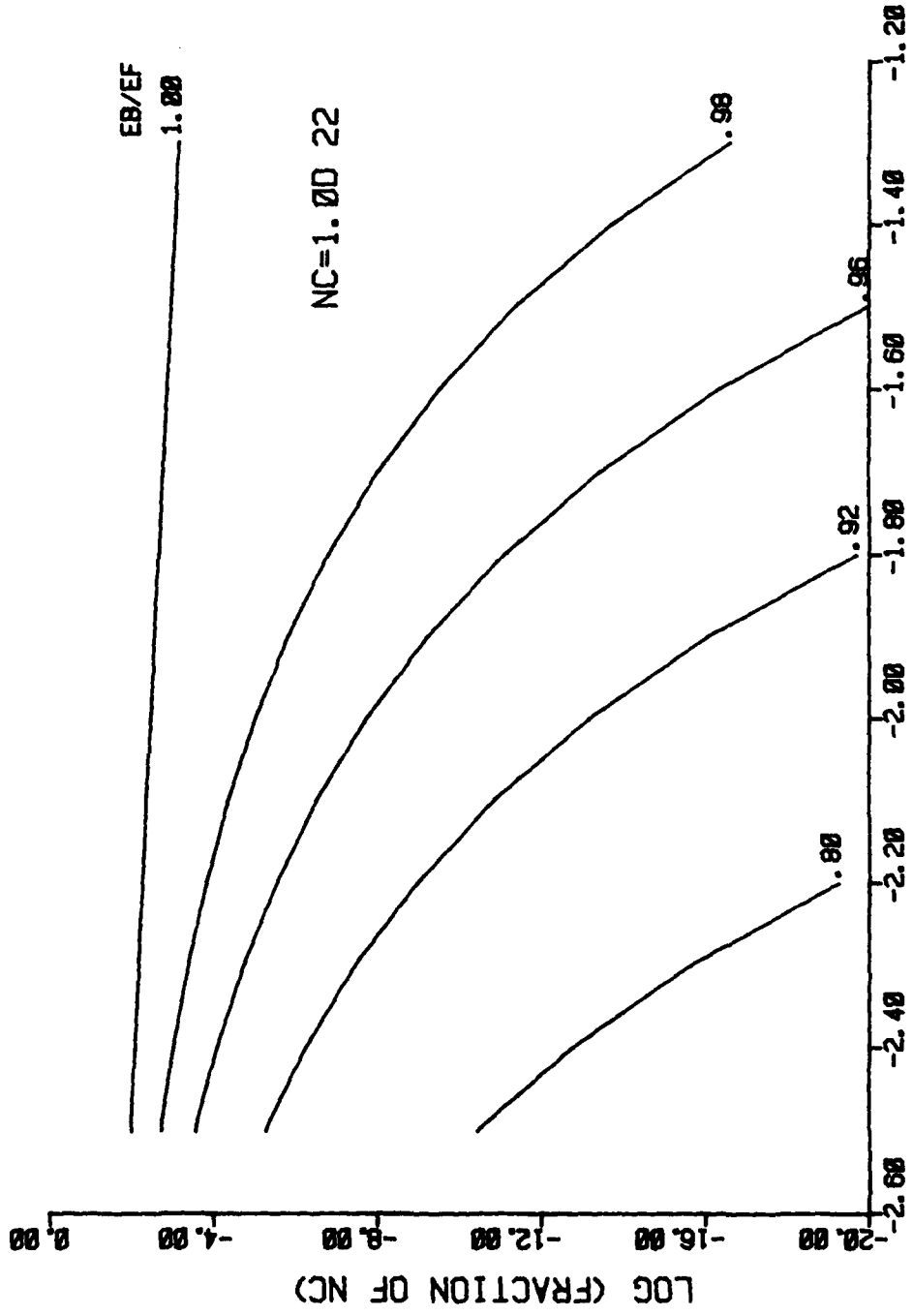

Fig.9 Density of Unoccupied Energy States Between the Conduction Band Edge and an Energy E_b where $E_c < E_b < E_f$

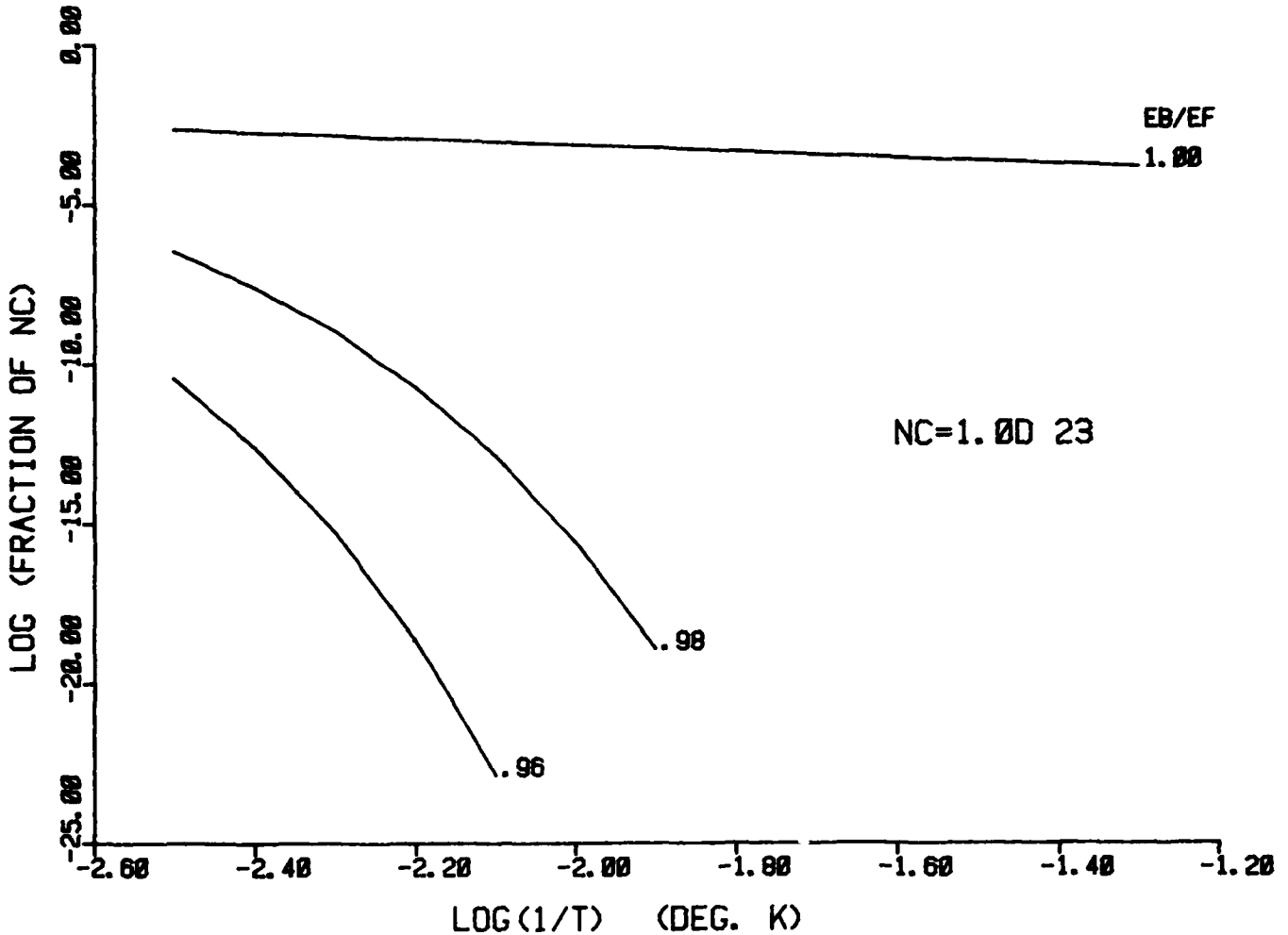

Fig.10 Density of Unoccupied Energy States Between the Conduction Band Edge E_c and an Energy E_b where $E_c < E_b < E_f$

4.0 The Transition Energy in a Schottky Barrier

In the conduction band of a metal the density of unoccupied energy states between E and (E + ΔE) is given by

$$\Delta N = 8\pi\sqrt{2}\,(\sqrt{m}/h)^3\sqrt{E}\left[1 + \exp(E_f - E)/kT\right]^{-1}\Delta E\,. \qquad (1\text{-}10)$$

If, indeed, semiconductor valence band electrons are to enter this conduction band there must be a place for them to go. If the number of electrons attempting to enter this conduction band at an energy E exceed the density of unoccupied states, many could return and not contribute to the electric current. If, instead, the density of unoccupied states at an energy E exceeds the source of supply, all valence band electrons attempting to enter the metal conduction band will find a place to go, and will contribute to the barrier electric current.

Next we consider the density of semiconductor valence band electrons that are attempting to enter this metallic conduction band. From Fig.1, all valence band electrons at an energy in excess of E_b must have undergone thermal excitation. Because all energy eigenvalues of the wave equation become imaginary in the forbidden band, we assume a Boltzmann distribution adequately describes the density of electrons in this region of the structure [6].

$$\Delta N = N_v\left(\frac{m}{2kT}\right)^{1/2}\exp\left(-\frac{m v_x}{kT}\right)\Delta v_x\,. \qquad (1\text{-}11)$$

Here we describe the density of valence band electrons with an x-axis directed velocity between v_x and $(v_x + \Delta v_x)$ that are attempting to enter the metallic conduction band.

Clearly, if the density of unoccupied states, Eq.1-10, exceeds the density of excited valence electrons, Eq.1-11, all can enter the conduction band. If, instead, the available electrons with a velocity v_x exceed the number of available unoccupied energy states, many will return to the valence band. For the purpose of this analysis we define a transition energy E_t. The transition energy is that energy bounding these two forementioned energy regions. At energies above E_t the rate at which electrons enter the conduction band is determined by the Maxwellian distribution of valence electrons, Eq.1-11. At energies below E_t the rate at which electrons enter the conduction band is determined by the availability of unoccupied energy states.

Figure 11 through Figure 14 illustrates the calculated value of E_t, described in terms of a barrier energy $W_c = (E_t - E_b)$. Because this transition barrier energy is not unlike the classical Schottky interface energy barrier W_c where $W_c = E_f - E_b$, we have related the two in these illustrative calculations. Classical theory is based upon an assumption that excited valence electrons must reach an energy E_f to enter the conduction band; this is equivalent to the general concept that a hole at E_f moves to E_b. Contrasting with this classical concept the transition barrier W_c represents the energy to which valence electrons must be excited for all to enter the conduction band. Below W_c their entry into the conduction band is governed by the availability of unoccupied energy states.

From these illustrations, Fig.11 through Fig.14, it is clear that the transition energy W_c is significantly lower than the classical barrier W_c, for all values of free electron density. It is through calculations of the

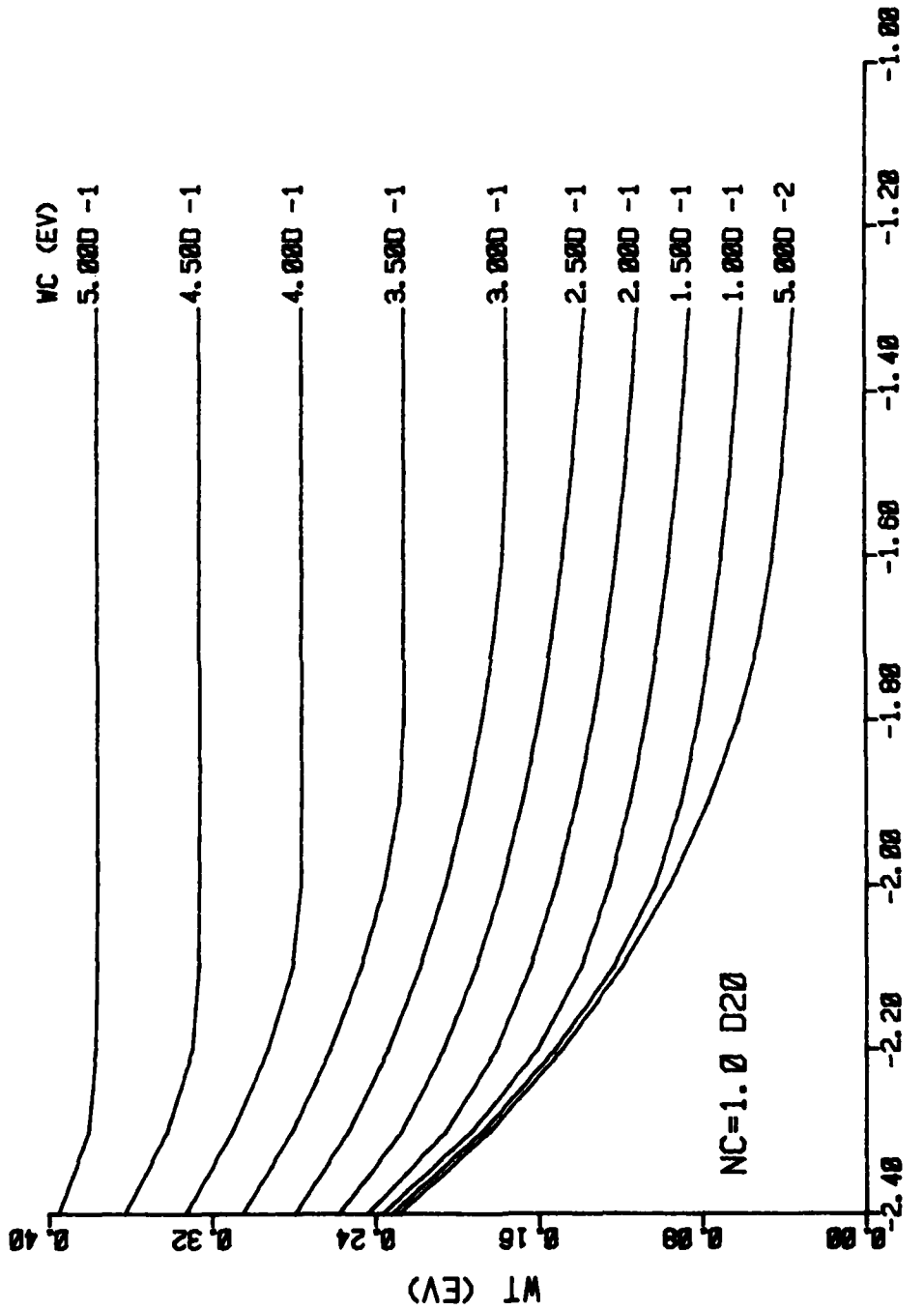

Fig.11 Calculated Transition Barrier W_t in a p-type Schottky Device

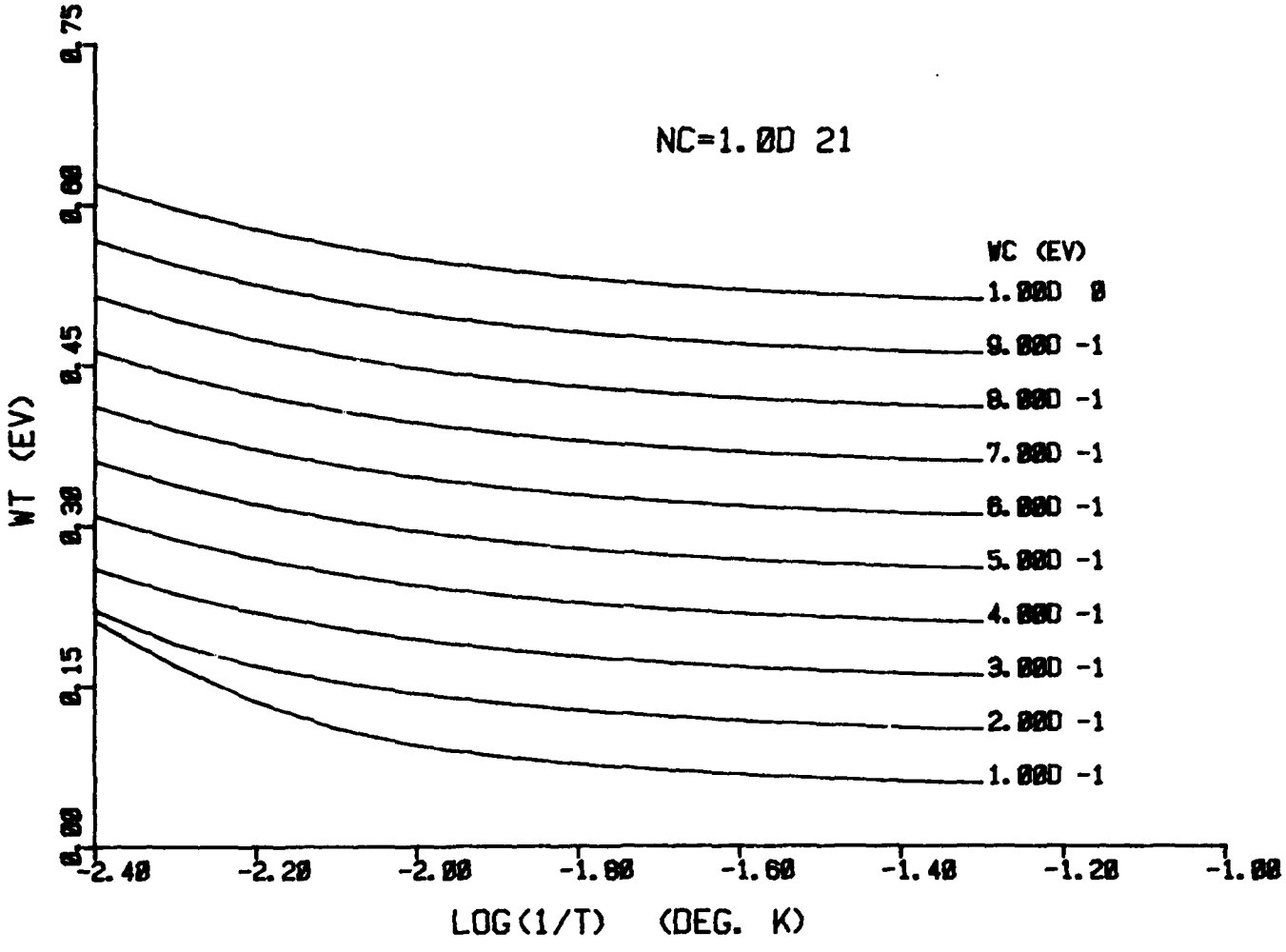

Fig.12 Calculated Transition Barrier W_t in a p-type Schottky Device

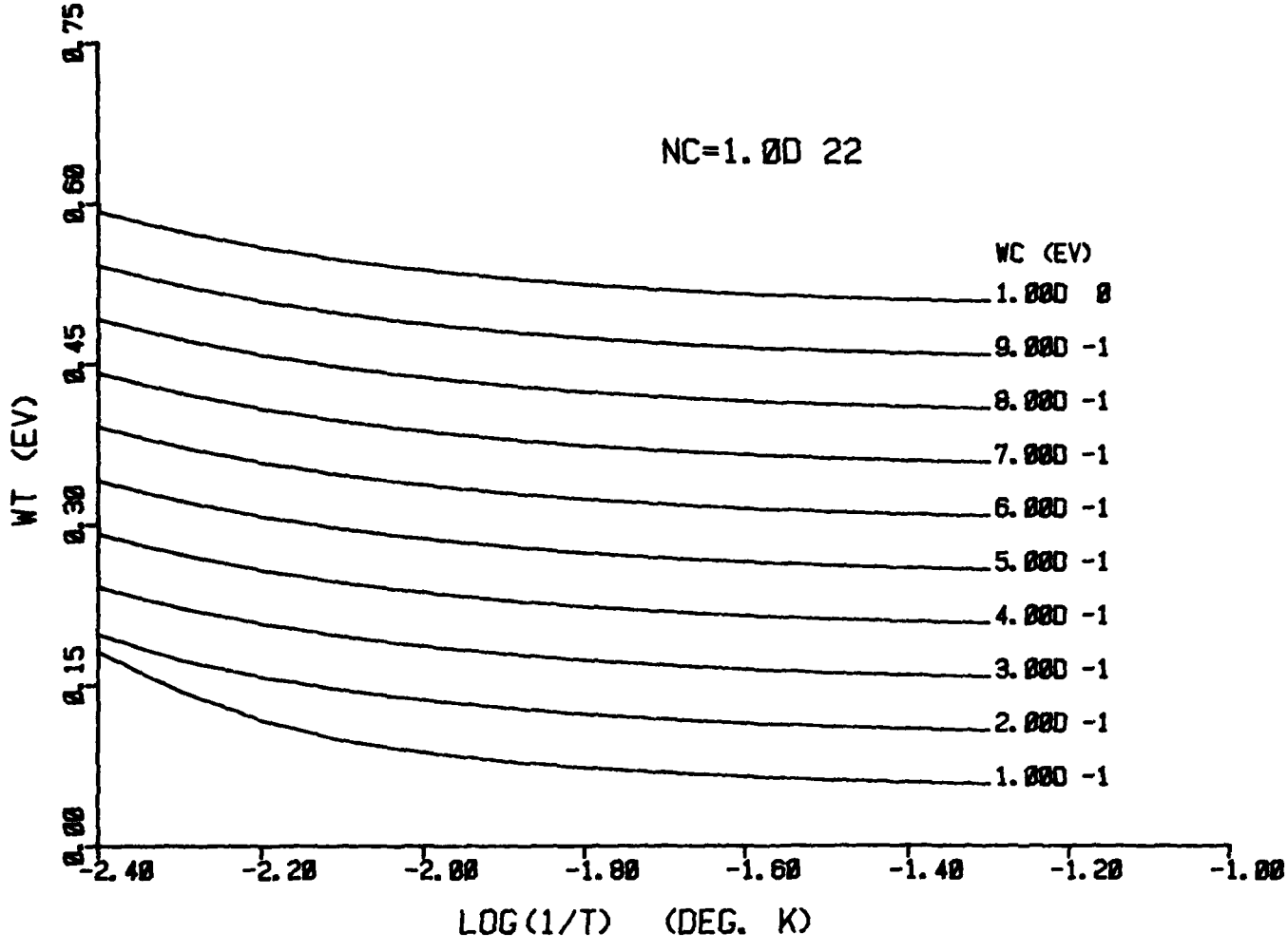

Fig.13 Calculated Transition Barrier W_t in a p-type Schottky Device

barrier electric current above and below the transition energy E_t we shall establish the reverse electric current in a p-type Schottky barrier.

5.0 The Electric Current in a Schottky Barrier---Classical Concept

The classical concept of p-type Schottky diode operation is that the total electric current can be represented by an expression of the form

$$J = J_o \left[1 - \exp \left(- q V_a / k T \right) \right] , \tag{1-12}$$

where V_a is an applied voltage and J_o is the saturation current.

To date, a rigorous calculation for J_o has not been found in the technical literature. It is an accepted practice to attribute J_o to two distinctly different mechanisms: first, hole-electron generation in the p-type semiconductor material and, second, hole transitions from the metal to the semiconductor material. The first mechanism can be acknowledged as well founded but, instead, there remains no real quantitative explanation for the saturation current at low temperatures; at temperatures that render hole-electron generation insignificant.

In order to adequately evaluate our concept of p-type device operation it is necessary to recast this classical theory into a form suitable for comparison. For this reason we abandon the notion of hole generation in the metal and consider this traditional theory in terms of valence electron excitation to the Fermi-level. Clearly, this is consistant with the concept of hole transitions from the Fermi-level to the valence band.

As in Section 4.0 of this chapter, we assume a Maxwellian velocity distribution for valence electrons given by

$$\Delta N = N_v \left(\frac{m}{2 \pi k T} \right)^{1/2} \exp \left(- \frac{1}{2} m v_x^2 / k T \right) \Delta v_x \tag{1-13}$$

Further, we assume an electric current produced by this velocity distribution given by

$$J_o = q \int_{v_f}^{\infty} v_x \, dn = q \, N_v \left(\frac{k \, T}{2 \, m^*} \right)^{1/2} \exp \left(-E_f / k \, T \right) , \qquad (1\text{-}14)$$

where

$$v_f = (2 \, E_f / k \, T) . \qquad (1\text{-}15)$$

Equation (1-14) represents an expression for the saturation current J_o that retains the traditional concept of hole transitions from the Fermi-level to the conduction band. Nonetheless, this expression has been developed in a manner that we believe is quantitatively reasonable, and can be used for comparison with new concepts of device operation arising from the present research.

In the foregoing equations N_v represents the density of valence electrons that are at an energy in excess of the valence band edge at the metal-semiconductor interface, E_b. This is easily calculated if we first determine the location of E_v, relative to the lower edge of the valence band.

The density of occupied energy states in a semiconductor is given by

$$N = 8\pi \sqrt{2} \left(\frac{\sqrt{m}}{h} \right)^3 \left(\frac{m^*}{m} \right)^{3/2} \int_o^{E_v} \frac{\sqrt{E} \, dE}{1 - \exp (E - E_f) \, k \, T} . \qquad (1\text{-}16)$$

If we assume a temperature of zero degrees K, the Fermi-level is essentially at E_v, and we have

$$N_t = 8\pi\sqrt{2}\left(\frac{\sqrt{m}}{h}\right)^3\left(\frac{m^*}{m}\right)^{3/2}\frac{3}{2}\;E_{f0}^{-3/2} \tag{1-17}$$

where N_t is the total number of valence electrons, and E_{f0} is the Fermi-level (at 0° K) as measured with respect to the lower boundary of the valence band. Because at the interface E_{f0} and E_b coincide, we can now state that the density of unoccupied states in the valence band is

$$N_v = \frac{3}{2}\;E_{f0}^{-3/2}\int_0^{E_{f0}}\frac{\sqrt{E}\;\;dE.}{1+\exp\left(E_f' + E\right)/kT} \tag{1-18}$$

where E_f' is the interface Fermi-level when measured with respect to the lower edge of the semiconductor conduction band,

$$E_f' = E_{f0} + (E_f - E_b) \tag{1-19}$$

Because valence electrons not found in the valence band must be at an energy in excess of E_b, we know the number of electrons involved in the Maxwellian distribution and, hence, N_v for Eqs.(1-12) and(1-13).

6.0 Reverse Current From Transitions Above E_t

As outlined in Section 4.0, electron excitation from the valence band E_b, Fig.1, to an energy above E_t (the transition energy) will assure a transition into the metal. Hence, like the traditional theory, we can immediately establish this component of the diode saturation current through a minor

modification of Eq.1-14.

$$J_1 = q \int_{v_t}^{\infty} v_x dn = qN_v \left(\frac{k\,T}{2\pi m}\right)^{\frac{1}{2}} \exp\left(-E_t/k\,T\right) \qquad (1\text{-}20)$$

where

$$v_t = (2\,E_t / m)^{\frac{1}{2}} \qquad (1\text{-}21)$$

This expression has been used in all of the following calculations as one component of the total saturation current J_o, and N_v is determined using Eq.1-18.

7.0 Reverse Current From Transitions Below E_t

Below the transition energy E_t the density of unoccupied energy states becomes less than the number of electrons available to occupy these states. If we recast the density of unoccupied states into an expression for electron velocity, Eq.1-10, we obtain

$$\Delta N = N_c \frac{3}{2} (E_{f0} / m)^{-3/2} v^2 \left[1 + \exp\left(E_f - \frac{1}{2} mv^2\right)\right]^{-1} dv \qquad (1\text{-}22)$$

Thus, the electric current produced by transitions to these energy states is given by

$$J_2 = q\,N_c \frac{3}{2} (E_{f0}/m)^{-3/2} \int_0^{v_t} \frac{v^3\,dv}{1 + \exp\left(E_f - \frac{1}{2} v\right)} \qquad (1\text{-}23)$$

where

$$v_t = (2\ E_t / m)^{\frac{1}{2}} \qquad (1\text{-}24)$$

Rewriting Eq.1-19 into energy we obtain

$$J_2 = 3qN_c\ E_{f0}^{-3/2}\ \ m^{-1/2} \int_0^{E_t} \frac{E\ \ dE}{1 + \exp\ (E_f - E) / k\ T}. \qquad (1\text{-}25)$$

Equation (1-21) is the expression we use for calculating the electric current produced by electron transitions below the transition energy E_t.

8.0 Computations of Reverse Electric Current

Few, if any, of the foregoing equations can be evaluated on an analytical basis; integration of the Fermi-Dirac distribution equation must be done numerically, on a computer. For this reason, our initial evaluation of this new concept of Schottky barrier operation has been accomplished through a sequence of electric current calculations. Equation (1-20) and Eq.(1-25) have been used for calculating the current predicted by these new theoretical concepts, and such calculations are compared with those using Eq.1-14 as representative of the classical theory for Schottky diode operation.

Figure 15 through 18 illustrate the total reverse current predicted by Eq.(1-20) and Eq.(1-21) for J_1 and J_2 respectively, throughout a wide assumed range for the free electron density in the metal conduction band. A comparison is first undertaken between these calculations Fig.15 through Fig.18, and similar calculations based upon classical theory, Fig.19 and Fig.20. Because W_c is given in these calculations ($W_c = E_f - E_b$), classical

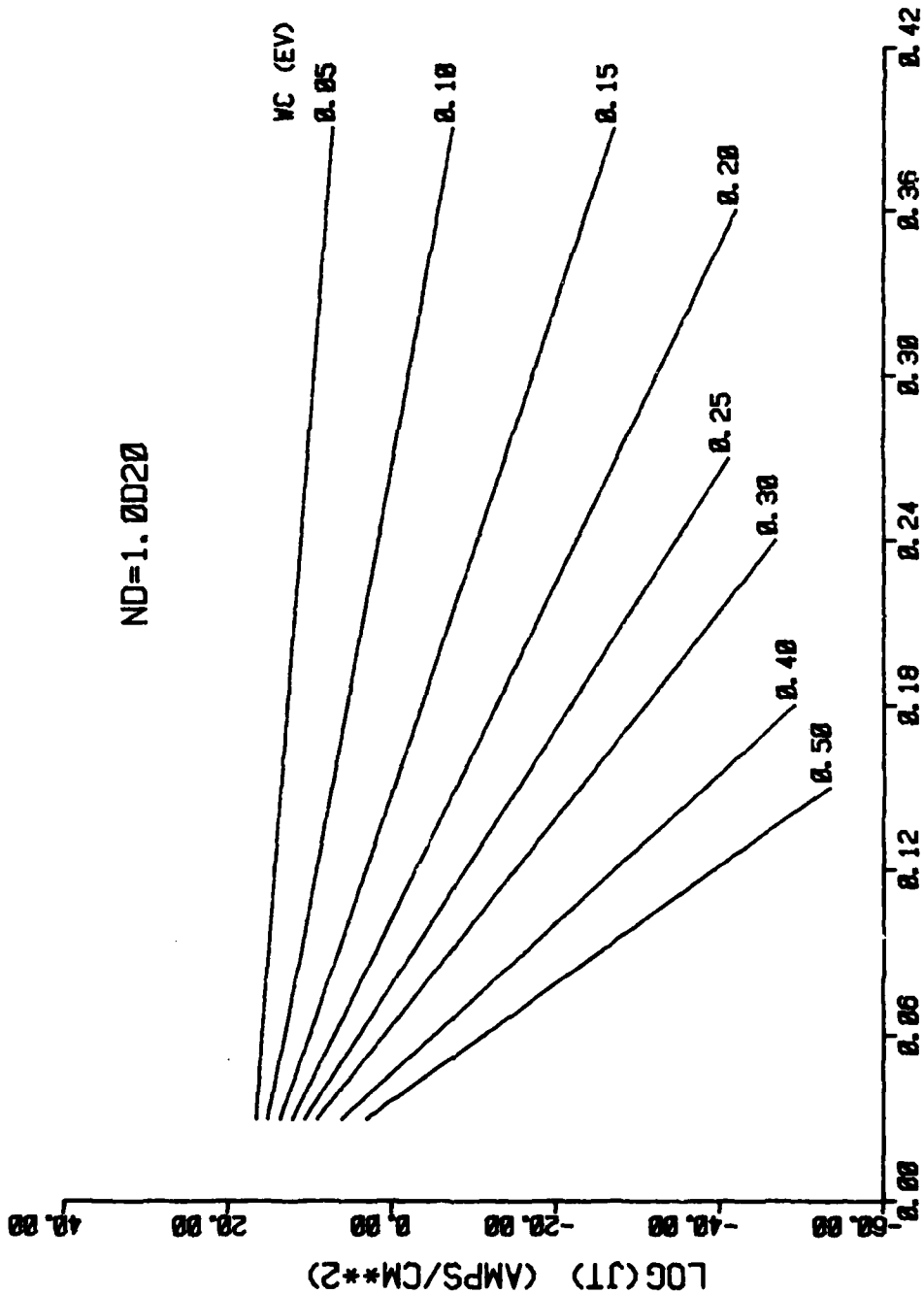

Fig.14 Calculated Total Saturation Current for a Range of Assumed Barrier Height, W_c

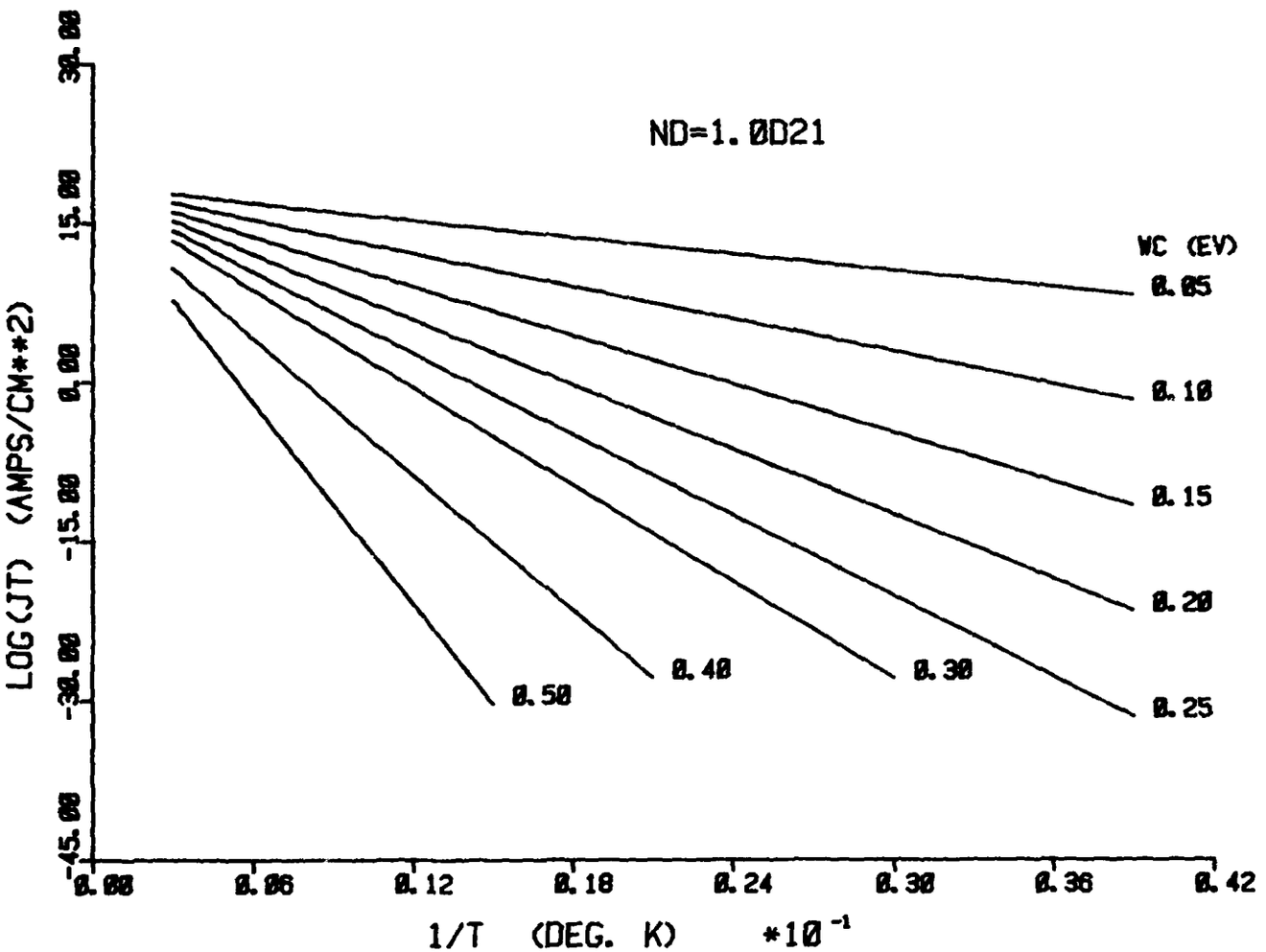

Fig.15 Calculated Total Saturation Current for a Range of Assumed Barrier Height, W_c

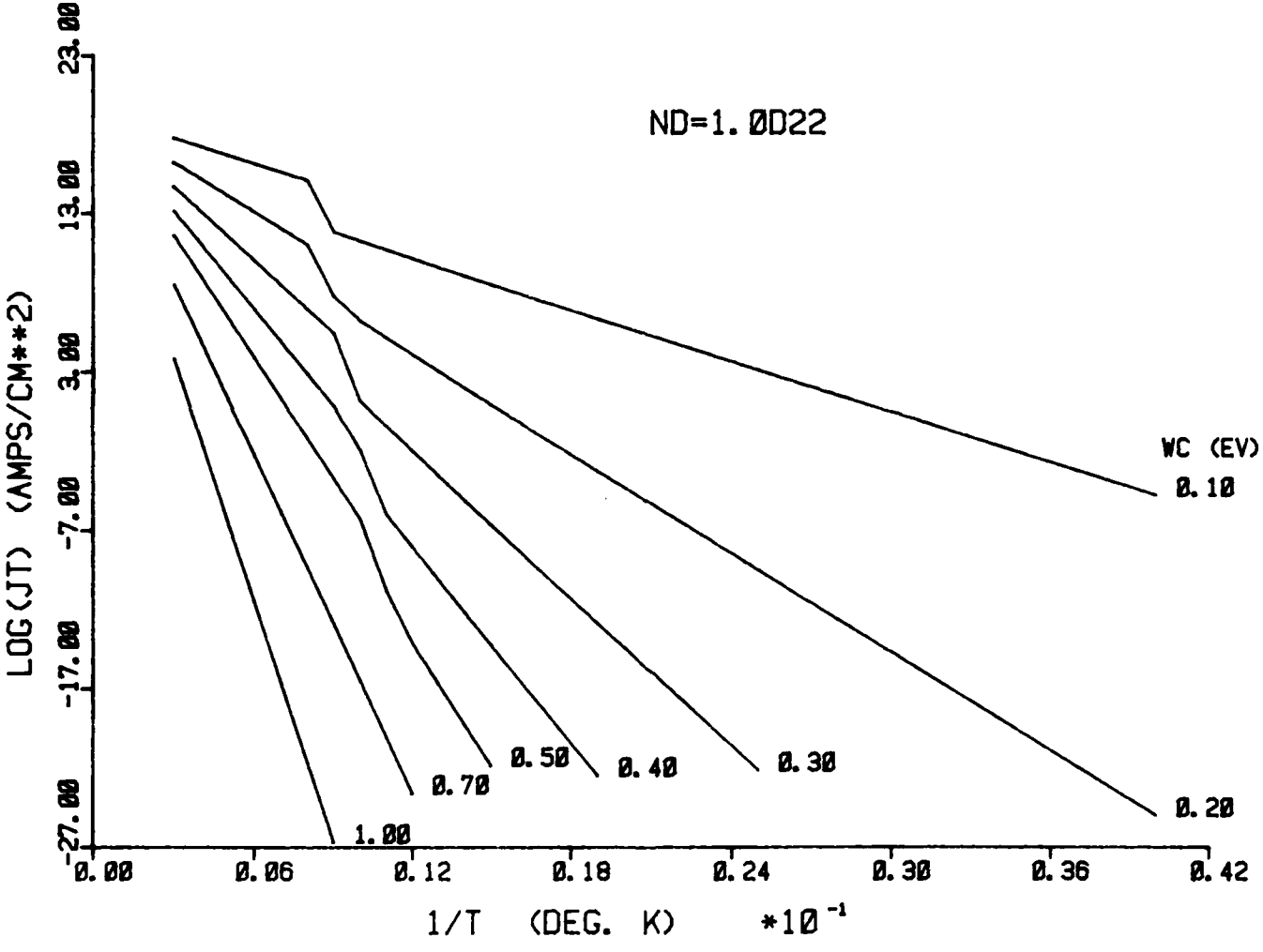

Fig.16 Calculated Total Saturation Current for a Range of Assumed Barrier Height, W_c

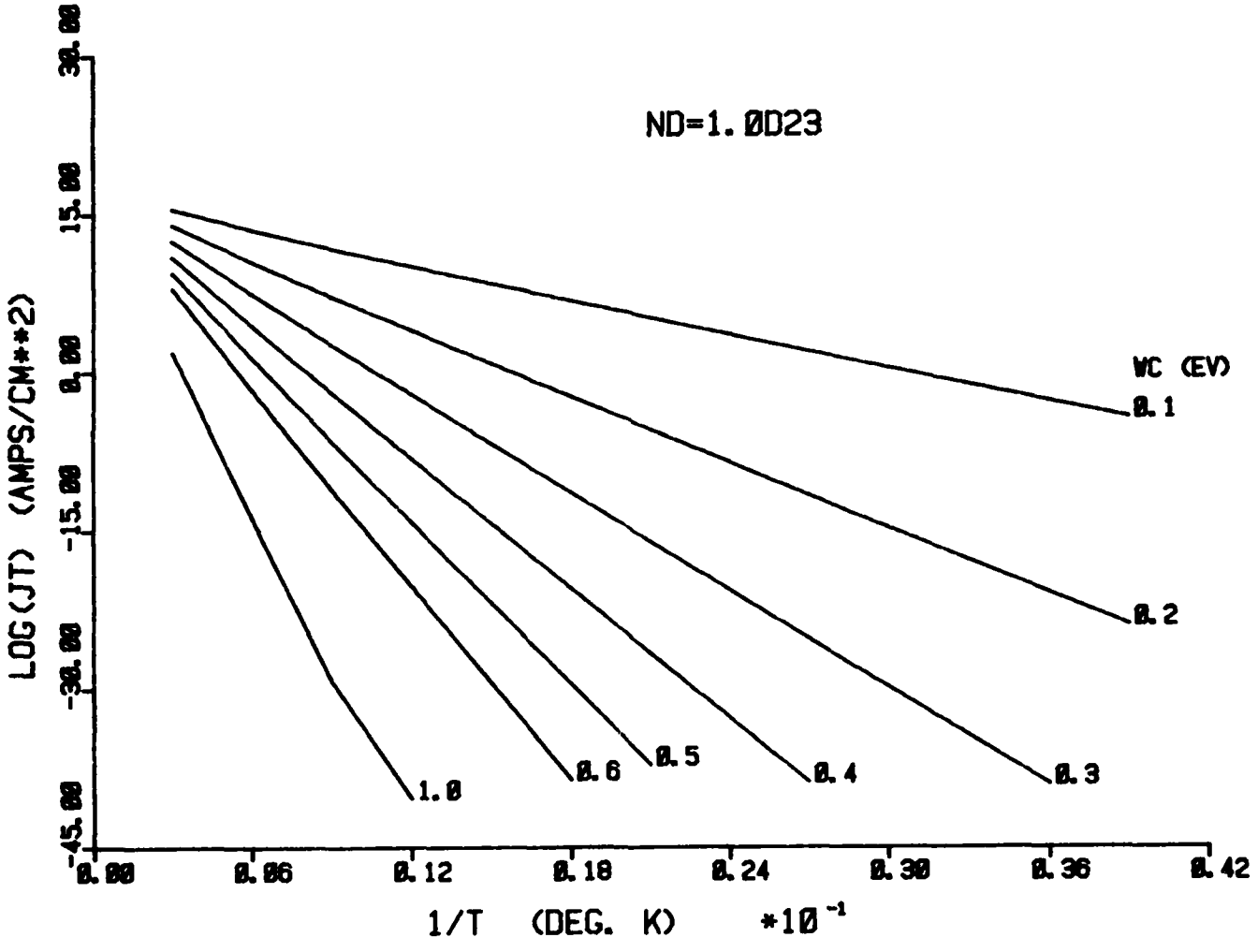

Fig. 17 Calculated Total Saturation Current for a Range of Assumed Barrier Height, W_c

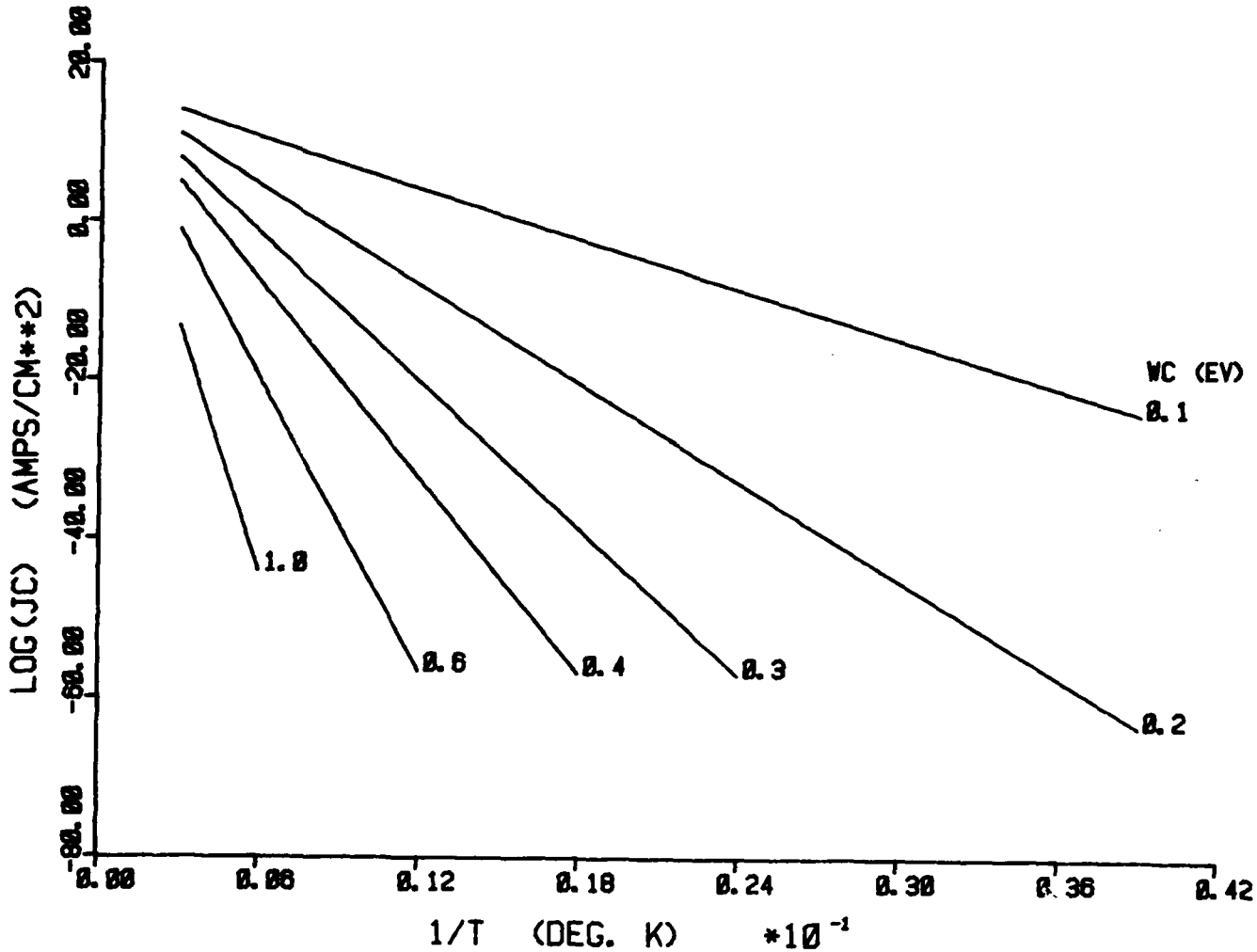

Fig. 18 Calculated Diode Current Using Classical Theory

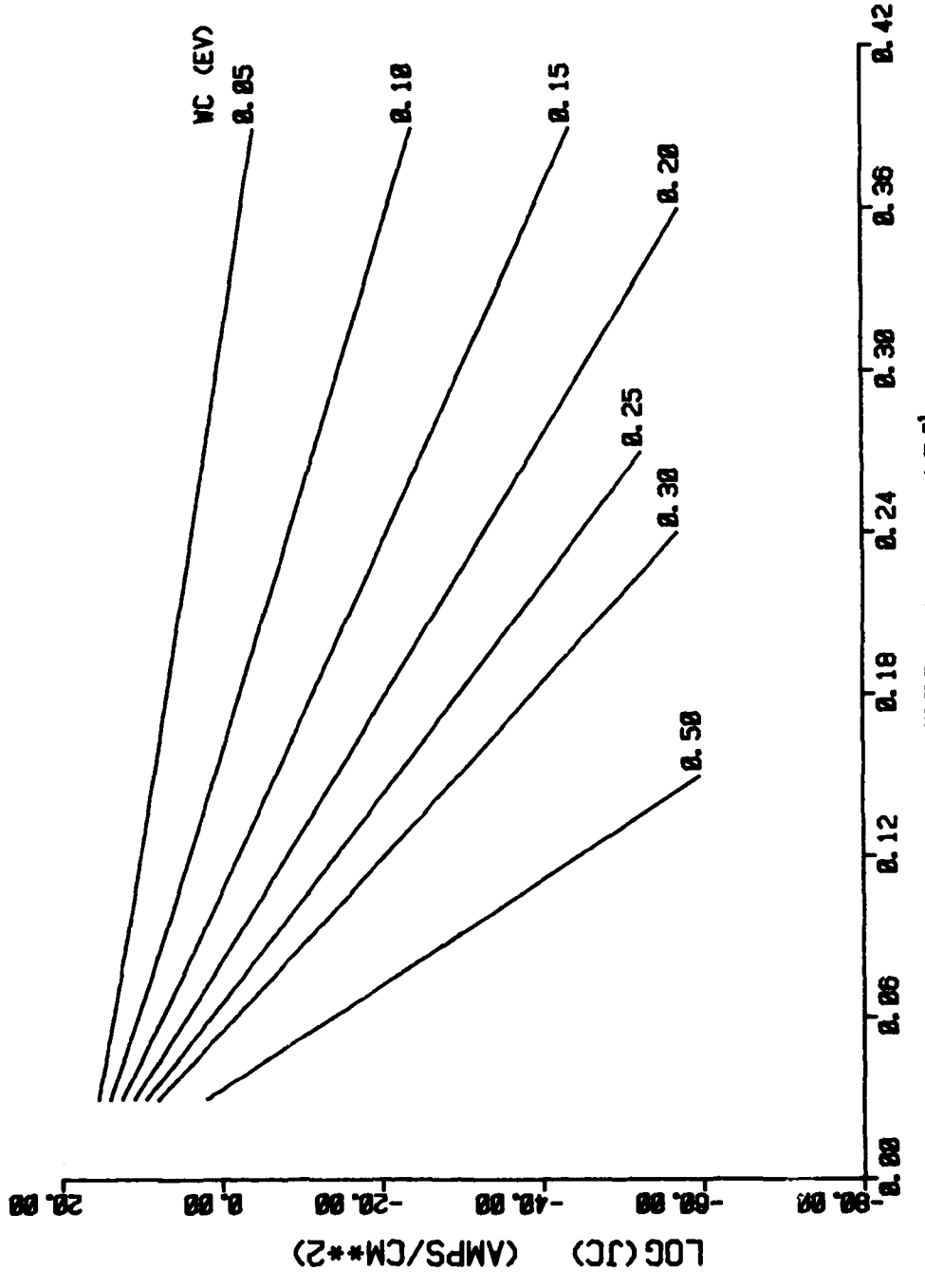

Fig.19 Calculated Diode Current Using Classical Theory

theory is nearly independent of the free electron density in the metal and, hence, only a single illustration is needed for J_c. For convenience, J_c is presented in two illustrations, Fig.19 and Fig.20, which have different assumed ranges for W_c.

We encounter two different situations in these calculations with relation to N_c, the conduction band electron density: first, when N_c is small ($N_c \approx 10^{20}$) and, second, when N_c is large ($N_c \approx 10^{23}$). When N_c is small the metallic conduction band closely resembles that of a highly degenerate n-type semiconductor; the Fermi-level is only a small distance above the conduction band edge, E_c. As a consequence, many of the assumed values for barrier energy W_c places the semiconductor valence band edge, E_b, below the conduction band edge, E_c. In the second case ($N_c \approx 10^{23}$) we have a metallic conductor in which the Fermi-level is well above the conduction band edge and, therefore, any reasonable assumption for W_c ($W_c \leq \approx 1.0$ ev) places the semiconductor valence band edge at the interface, E_b, *well within the metal conduction* band ($E_c \leq E_b \leq E_f$).

Calculations show that by assuming $N_c = 10^{20}$, this new theory of operation yields a reverse current, J_t, that is always substantially larger than that given by classical theory, J_c. For purposes of comparison, some illustrative calculations yield at T = 60° K:

W_c (ev)	J_t (amps/cm^2)	J_c(amps/cm^2)
0.5	10^{-53}	10^{-60}
0.3	10^{-23}	10^{-29}
0.25	10^{-15}	10^{-22}
0.2	10^{-8}	10^{-14}

Because in the foregoing calculations E_b lies below the conduction band edge no contribution to J_t arises from direct electron transitions from the valence band to the conduction band; all transitions are due to thermally excited valence electrons with an energy in excess of E_b. For $N_c = 10^{20}$(cm^{-3}),

only at an assumed barrier of .05 ev ($W_c = 0.05$) does this direct transition mechanism produce an electric current, J_2, that contributes significantly to J_t, Fig.25. For this low barrier situation ($W_c = 0.05$ ev) we calculate:

T(°K)	J_1	J_2	J_t	J_c
27	$10^{5.5}$	$10^{7.9}$	$10^{7.9}$	$10^{-4.2}$
30	$10^{6.3}$	$10^{8.7}$	$10^{8.7}$	$10^{-2.7}$
33	$10^{7.1}$	$10^{9.4}$	$10^{9.4}$	$10^{-1.1}$
41	$10^{7.9}$	$10^{10.2}$	$10^{10.2}$	$10^{4.0}$
47	$10^{8.7}$	10^{11}	10^{11}	10^{19}
55	$10^{9.6}$	$10^{11.8}$	$10^{11.8}$	10^{35}
66	$10^{10.4}$	$10^{12.5}$	$10^{12.6}$	10^{51}

Contrasting with the foregoing small free electron situation, by assuming $N_c = 10^{23}$ (cm^{-3}) the Fermi-level is moved well away from the conduction band edge. As with $N_c = 10^{20}$ we again obtain a small electric current component due to direct transitions, but for an entirely difernt reason. Setting $N_c = 10^{23}$ places the interface valence band energy, E_b, well within the metallic conduction band edge which, under the proper circumstances, could produce a large direct transition current. When $N_c = 10^{23}$ we find that unoccupied conduction band energy states are clustered within a small energy range from E_f. As a consequence, when E_c is sufficiently large we obtain a negligible amount of current due to direct electron transition from the valence band to the conduction band.

For the purposes of illustration, the following represent the calculated electric current at T = 83° k:

W_c (ev)	J_t	J_1	J_c
0.6	10^{-20}	10^{-20}	10^{-56}
0.5	10^{-14}	10^{-14}	10^{-32}
0.3	10^{-2}	10^{-2}	10^{-20}
0.2	10^{4}	10^{4}	10^{-8}
0.1	10^{10}	10^{10}	10^{-4}

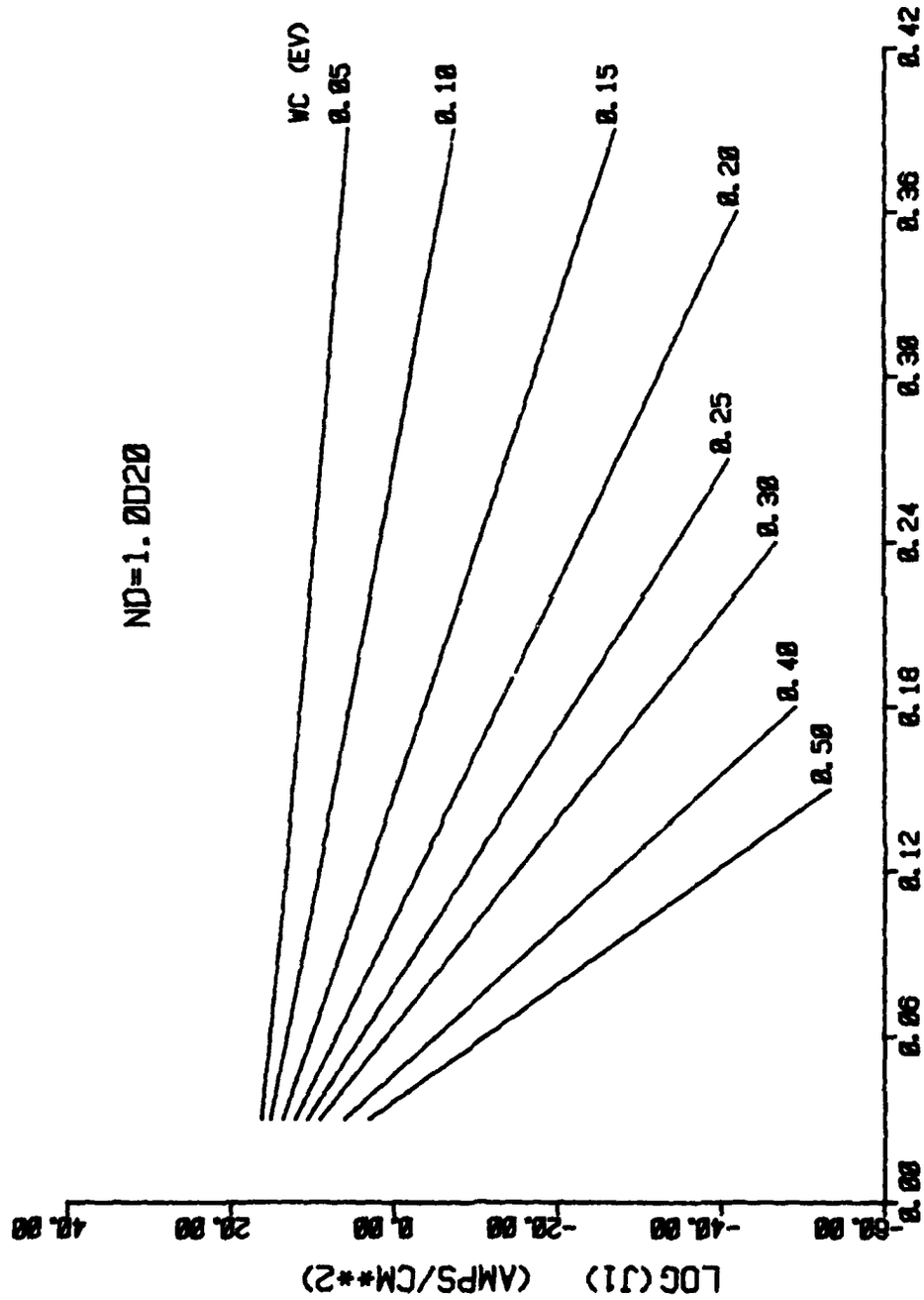

Fig.20 Saturation Current Component Due to Transition of Electrons with an Energy Greater Than E_t

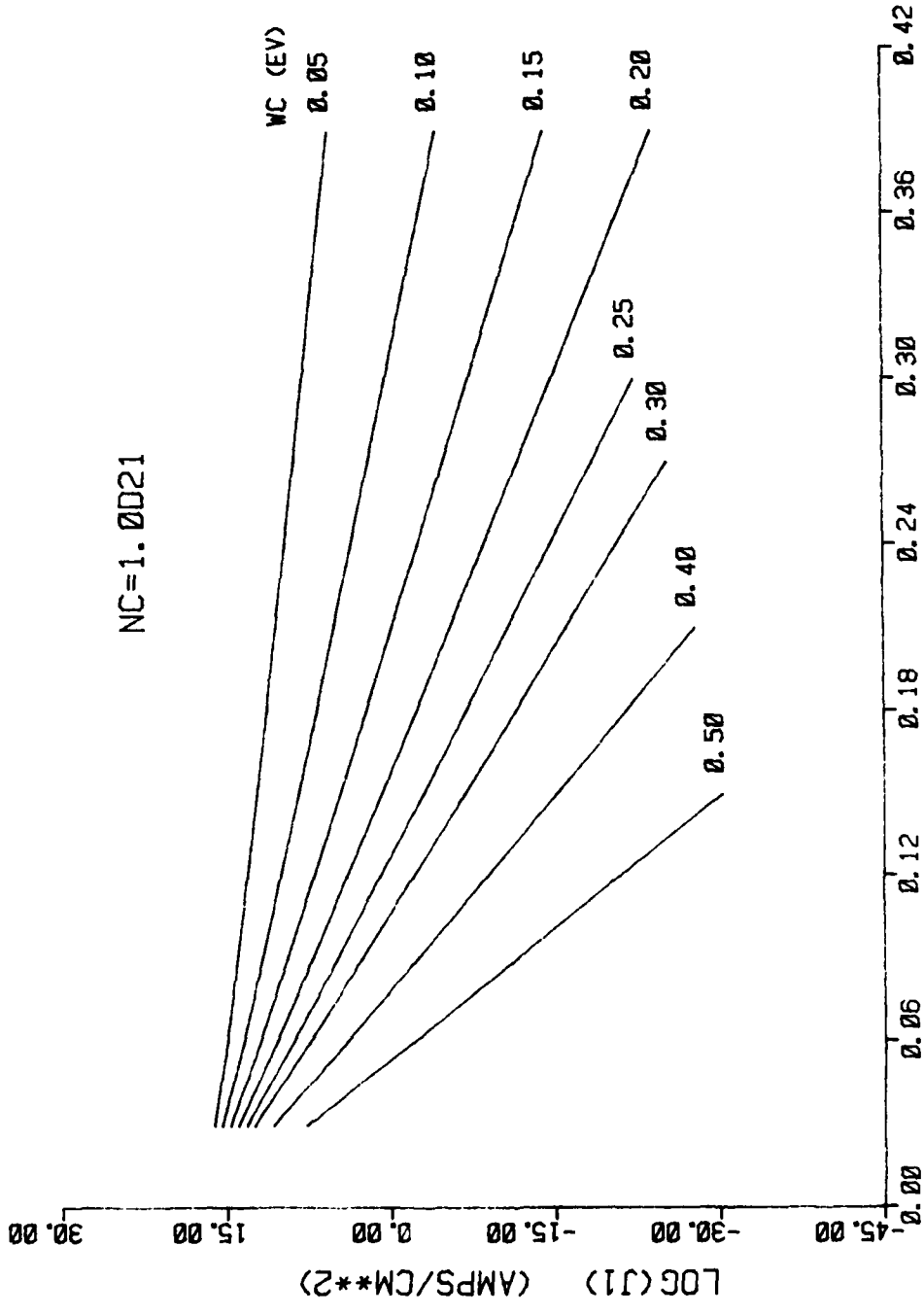

Fig. 21 Saturation Current Component Due to Transition of Electrons with an Energy Greater Than E_t

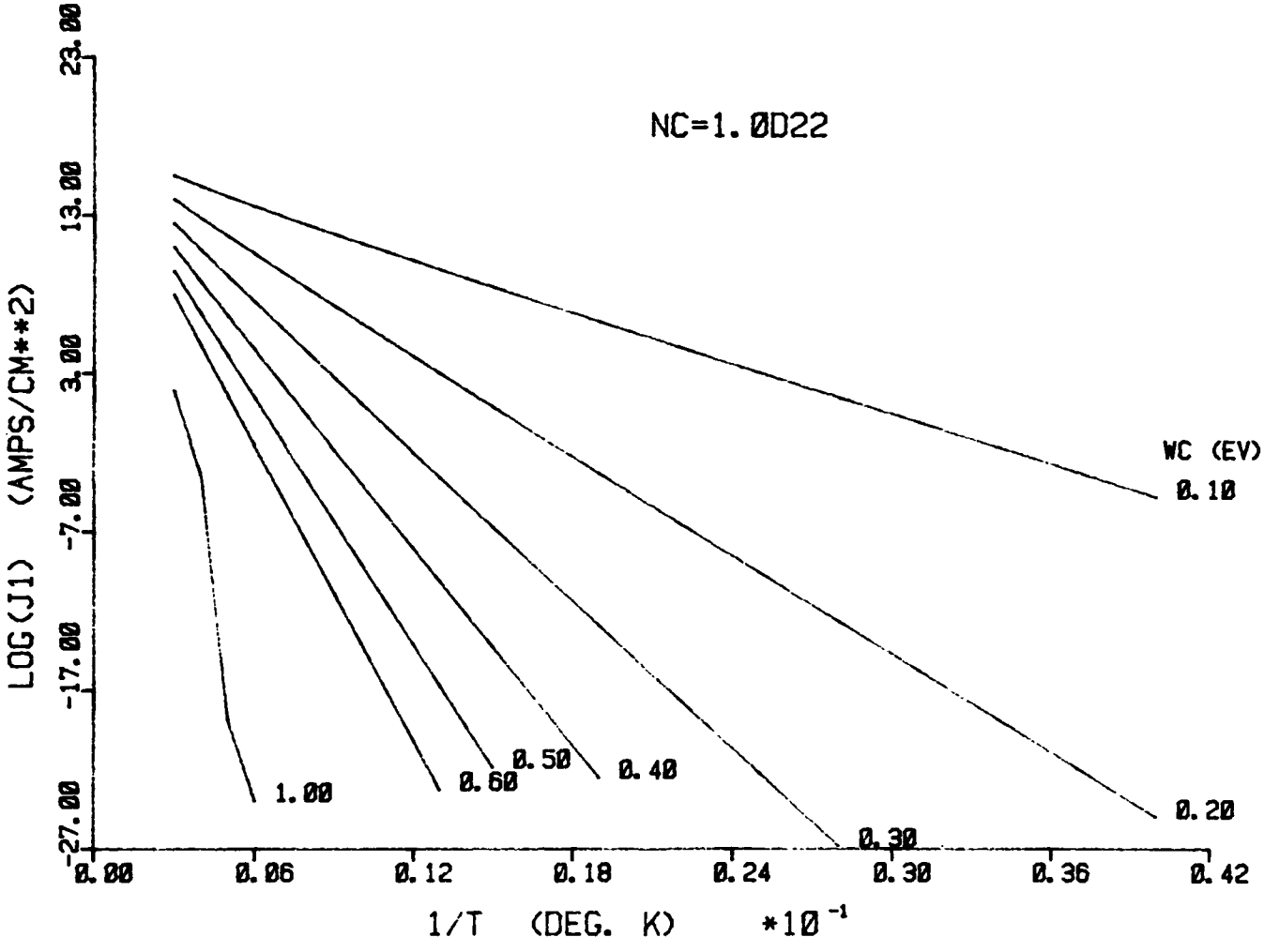

Fig. 22 Saturation Current Component Due to Electrons with an Energy Greater Than E_t

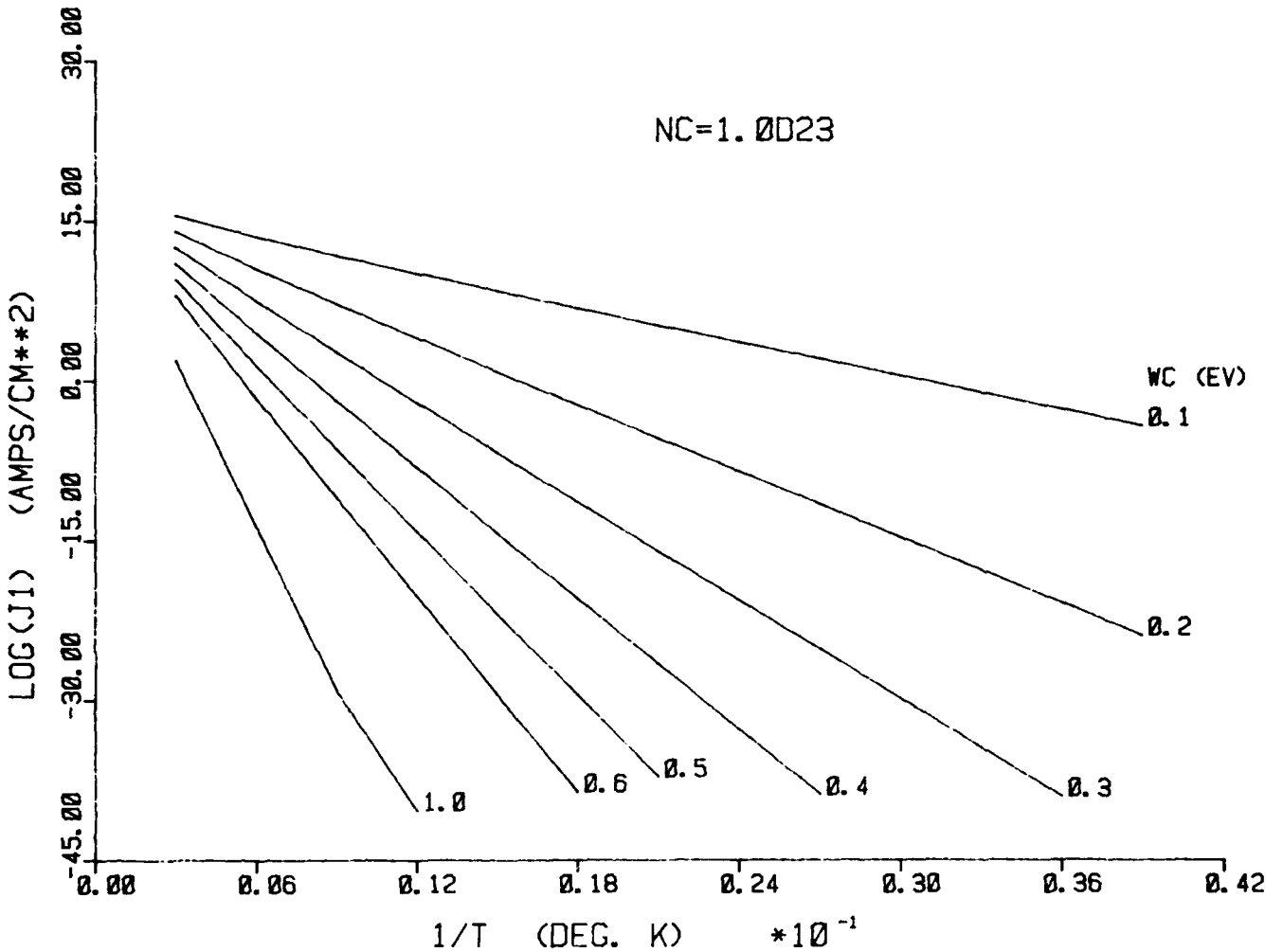

Fig.23 Saturation Current Component Due to Electrons with an Energy Greater Than E_t

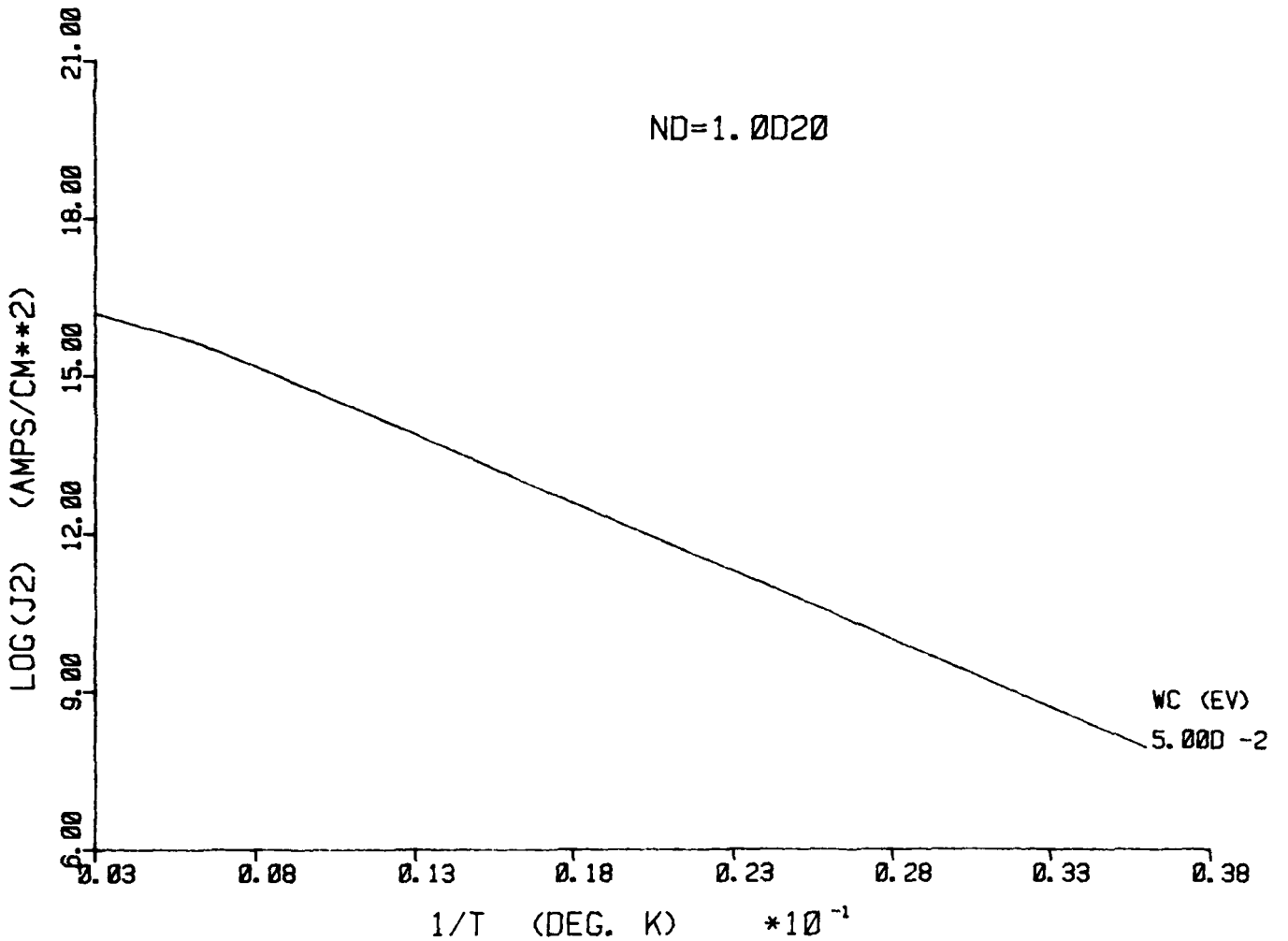

Fig. 24 Saturation Current Component Due to Transitions by Electrons with an Energy Less Than E_t

where current is in amps/cm^2. In all of these calculations the direct transition current remained relatively unchanged at 10^{-47} amps/cm^2; this situation probably arises from underflow protection within the computer program. This sequence of calculations indicate that very few unoccupied states reside in lower regions fo the conduction band when $N_c = 10^{23}$. Nonetheless, a sufficient number exist below E_f so that J_t is significantly larger than J_c.

An intermediate range is found between $N_c = 10^{20}$ and $N_c = 10^{23}$ where both J_1 and J_2 can contribute in a significant fashion to the total electric current. In this intermediate region, where $10^{20} < N_c < 10^{23}$, the unoccupied energy states can reside at energy levels far below the Fermi-level, E_f. As a consequence of this situation the transition energy E_t can reside well below E_f and, therefore, $W_t < W_c$, which assures $J_c < J_1$. Additionally, a large number of unoccupied energy states can reside below the transition barrier W_t, and this situation implies a direct transition current J_2 that can be significant.

We first consider the electric current calculated for an assumed free electron density N_c of 10^{21} (cm^{-3}). At 66° K our calculations yield the following results:

W_c (ev)	J_t	J_1	J_2	J_c
0.30	10^{-5}	10^{-6}	10^{-5}	10^{-29}
0.20	$10^{2.8}$	$10^{0.8}$	$10^{2.8}$	10^{-14}
0.10	10^{10}	$10^{8.4}$	10^{10}	$10^{0.8}$

where all current is in amps/cm^3. In this situation two different (although related) mechanisms contribute to the total electric current J_t. Transitions of thermally excited electrons to unoccupied energy states produce an electric current component J_1 that is significantly greater than predicted from classical concepts, J_c. This situation implies that the transition to unoccupied energy states below E_f ($E_t \leq E \leq E_f$) occurs at a greater rate than transition to unoccupied states above E_f ($E_f \leq E \leq \infty$). These calculations also show that transitions with no apparent thermal excitation

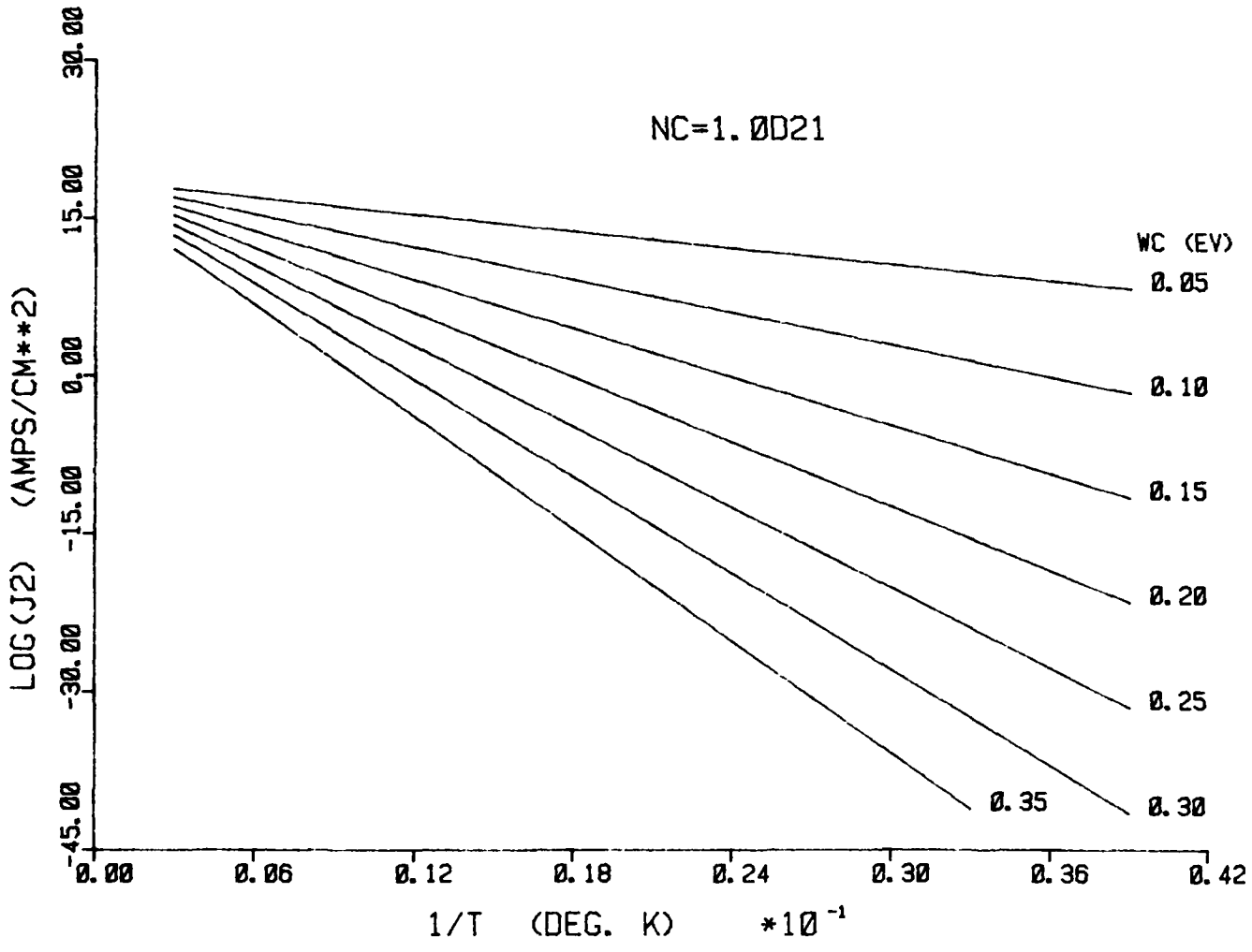

Fig.25 Saturation Current Component Due to Transitions by Electrons with an Energy Less Than E_t

($E_c \leq E \leq E_t$) take place at a rate that is significantly greater than the transition of thermally excited valence electrons. Hence, in this computational illustration both J_1 and J_2 are significant in magnitude, and in combination they produce a greater electric current than predicted using classical concepts of diode operation.

By assuming $N_c = 10^{22}$ (cm^{-3}) we obtain a Fermi-level that is well above the conduction band edge, yet the distribution of unoccupied states extends for a significant energy range below this Fermi-level. As a consequence, direct transition current J_2 can be very large, Fig.26, in conjunction with a large current J_1 due to transitions above the transition energy E_t, Fig.23. In combination, the total junction current, Fig.17, is much larger than expected from conventional concepts of device operation, Fig.19 and Fig.20.

It should be mentioned that the apparent change of slope in Fig.17 appears to be a real mechanism, and not a problem of the computer program. At high temperature the total current is dominated by direct valence electron transitions to the conduction band and, thereby, determining the total current J_t. A decrease of temperature produces a rapid fall off of this direct transition current, Fig.27, and J_t is determined by transitions above the transition energy E_t. Although it is not shown in these calculations, at a lower temperature many of these curves in Fig.17 exhibit another change of slope; this change is attributed to a rapid decrease of N_v; the valence electrons residing above the valence band edge, E_b, at the metal-semiconductor interface.

9.0 Reverse Current in a p-type Schottky Barrier at 77°K

In reverse bias situations it is presumed that holes are generated at the metal-semiconductor interface through the foregoing mechanisms. After generation these holes move to charge neutral regions of the p-type

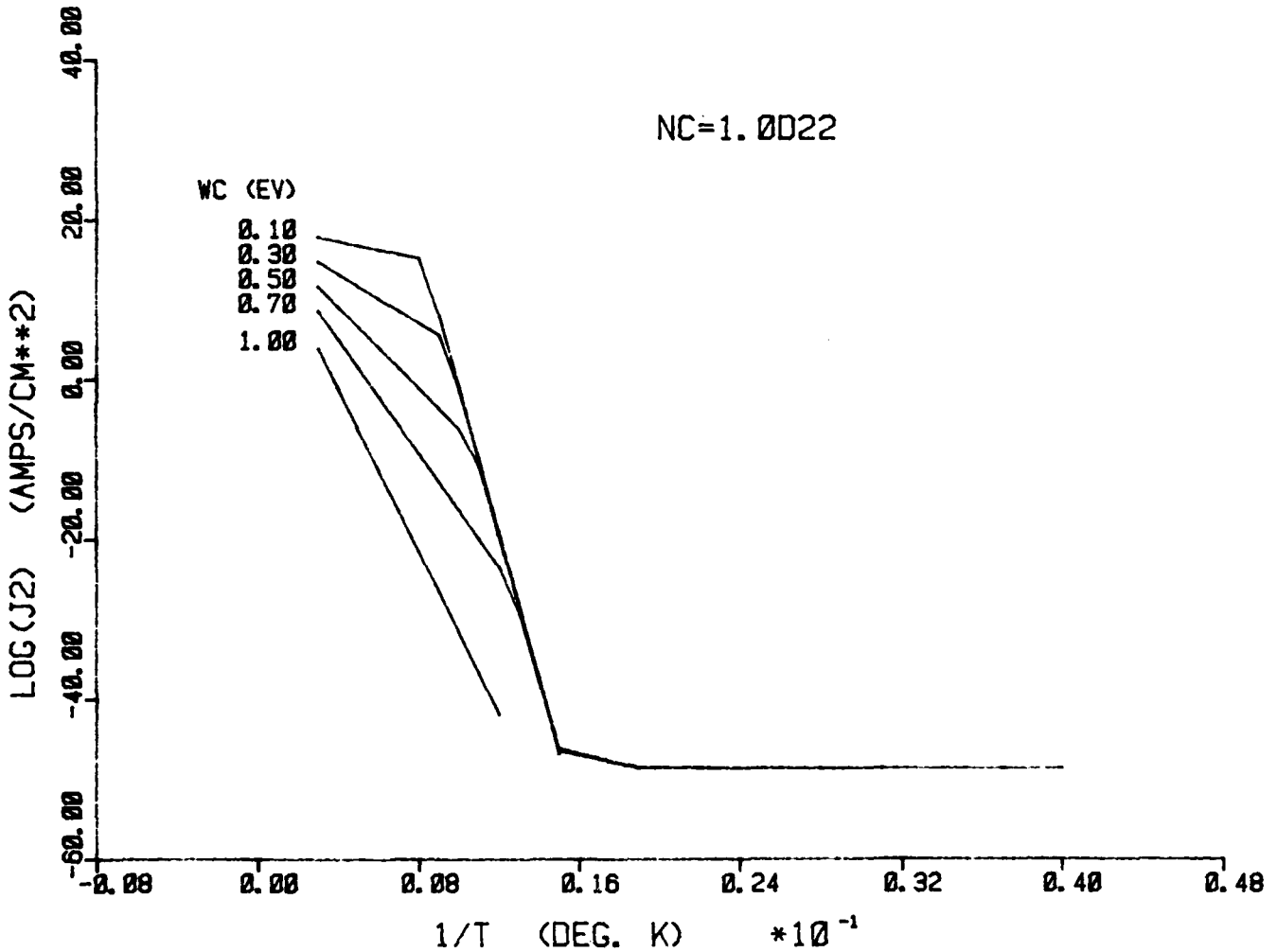

Fig.26 Saturation Current Component Due to Transitions by Electrons with an Energy Less Than E_t

material, under the influence of a space-charge electric field; thereby a reverse electric current is produced in this semiconductor device. Experiment shows that the magnitude of this reverse current increases with applied reverse voltage, and this mechanism has not yet been included in the present theory.

From conventional concepts of device operation it can be shown [6] that a lowering of the potential barrier results from the attractive forces between an interface generated hole, and an image charge at the metal. This mechanism is frequently called the Schottky effect, and through this mechanism E_b, Fig.1, will be increased by an amount

$$\frac{1}{2}\sqrt{\frac{q f_o}{\pi \epsilon_o}} \quad , \tag{1-26}$$

where f_o represents the space-charge layer electric field at the metal-semiconductor interface. Using the depletion approximation for determining this electric field, Eq.1-26 has been added to assumed values of E_b yielding a conventional interface energy barrier of

$$W_c = E_f - E_b - \frac{1}{2}\sqrt{q f_o / \pi \epsilon_o}. \tag{1-27}$$

We next apply our new theoretical concepts to a reverse biased Pt-Si diode operating at 77° K. Additionally, we compare the results of such calculations with similar calculations using conventional theoretical concepts. It is emphasized that little is known about the Pt-Si in this semiconductor device and, therefore, unknown parameters must be introduced by guess, rather than fact. Specifically, for this calculation we require the free electron density in the Pt-Si region, and the density

of states effective mass of these free electrons. For the latter we assume (m*/m) is equal to unity, which is indeed incorrect, but this parameter is unknown.

For the free electron density we have adjusted its magnitude to yield a reverse electric current typical of that obtained in experimental devices operating at 77° K. Our best guess is that the Pt-Si region contains a free electron density of approximately 10^{20} (cm^{-3}), which implies this region is more accurately classified as a degenerate semiconductor, rather than a metal. Figure 27 illustrates the calculated reverse electric current vs. applied voltage, assuming a free electron density between 10^{20} (cm^{-3}) and 1.5×10^{20} (cm^{-3}), assuming an energy barrier W_c of 0.27 (ev). Similarly, using conventional theoretical concepts the calculated reverse current is illustrated in Fig. 28; this calculated current is independent of the Pt-Si characteristics.

These calculations suggest that the reverse current of a p-type Pt-Si diode will be many orders of magnitude larger than predicted from traditional theoretical concepts. Further, implied by these calculations is that without good control over the fabrication processes poor reproductability might be expected in Pt-Si devices. For example, our calculated reverse current, at a given biasing voltage, changes by nearly two orders of magnitude for a free electron density between 10^{20} (cm^{-3}) and 1.5×10^{20} (cm^{-3}).

It can be shown that an assumed barrier W_c of 0.27 ev locates the valence band edge at the interface, E_b in Fig.1, below the conduction band edge, E_c. For this reason the mechanism of direct electron transition cannot take place between the valence band and the Pt-Si region of this device. Nonetheless, calculations show that the transition energy E_t lies close to the conduction band edge E_c yielding a true energy barrier of about $E_c - E_b$, rather than $E_f - E_b = 0.27$ (ev), as suggested by conventional theory. It is suggested that this significant difference between the assumed energy barrier and the true energy barrier produces the unexpected large reverse electric current in a Pt-Si diode.

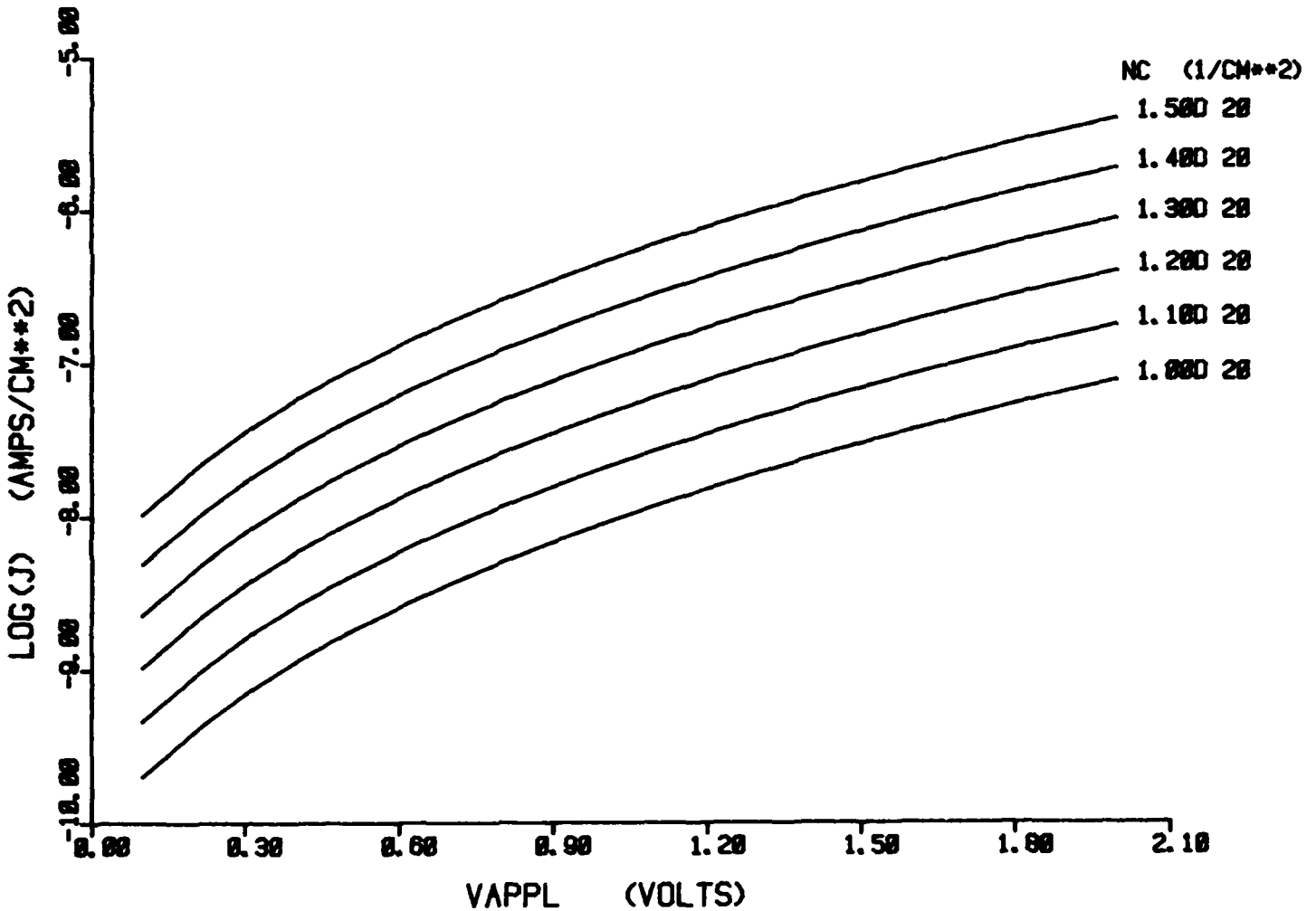

Fig.27 Calculated Volt-Ampere Characteristics Based Upon Results from this Research (Assumed Barrier W_c = 0.27 ev, T = 77°K)

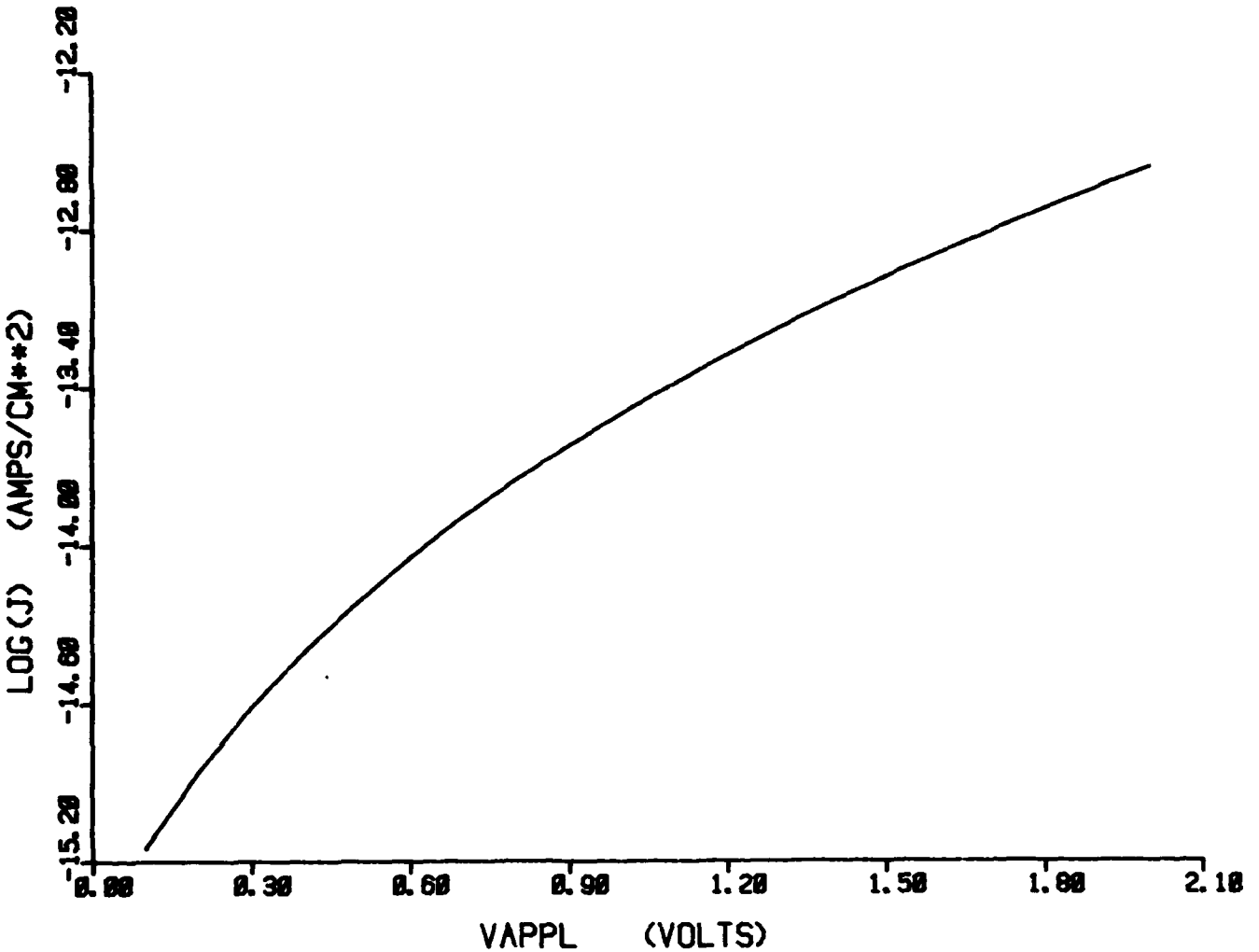

Fig.28 Calculated Volt-Ampere Characteristics of a Schottky Barrier Based upon Conventional Device Concepts (Assumed Barrier W_c = 0.27 ev, T = 77° K)

Chapter II

Potential Calculations for a Schottky Barrier Diode

1.0 Introduction

Most mathematical models of semiconductor device operation are based upon the concepts and mathematical equations outlined by W. Van Roosbroek[7] in 1950. In one spatial dimension, the steady-state form of these equations are given by:

$$\text{a)} \quad \frac{d^2\Psi}{dx^2} = -\frac{q}{k\,\epsilon_o}\,(N_D - N_A - n + p)$$

$$\text{b)} \quad J_p = -q\,D_p\,\frac{dp}{dx} - q\,\mu_p\,p\,\frac{d\Psi}{dx}$$

$$\text{c)} \quad J_n = q\,D_n\,\frac{dn}{dx} - q\,\mu_n\,n\,\frac{d\Psi}{dx} \qquad (2\text{-}1)$$

$$\text{d)} \quad \frac{dJ_p}{dx} = C_1$$

$$\text{e)} \quad \frac{dJ_n}{dx} = C_2$$

$$\text{f)} \quad J_T = J_p + J_n$$

Equation (2-1a) is Poisson's equation, and it relates the divergence of the electric field to the electrostatic charge distribution arising from both mobile charge carriers (holes p and electrons n), and immobile ionized impurity atoms within the semiconductor lattice.

Equations (2-1b) and (2-1c) give the electric current density arising from the transport of mobile holes and electrons. These equations express the dependency of each electric current component, J_p and J_n, upon the concentration gradient of holes and electrons, the mobility of these charge carriers, and the electric field within the semiconductor material.

Equations (2-1d) and (2-1e) are the continuity equations for holes and electrons in a semiconductor, and these equations contain unspecified rates of carrier generation and recombination.

Equation (2-1f) states that the total electric current density, J_T, is the sum of the electric current due to holes, J_p, and electrons, J_n.

Throughout this analysis we assume the applicability of Boltzmann statistics, and the hole and electron densities are given by

$$\text{a)} \quad n = n_i \exp -\left[q\left(\Psi - \phi_n\right) / kT\right]$$

$$\text{b)} \quad p = n_i \exp -\left[q\left(\phi_p - \Psi\right) / kT\right] \qquad (2\text{-}2)$$

where ϕ_n and ϕ_p are the quasi-Fermi potentials for electrons and holes, respectively.

The carrier generation/recombination term in Eqs.(2-1d) and (2-1e) is assumed composed of three terms: first, carrier generation/recombination through defects, second by impact and/or avalanche ionization and, third, hole generation through valence electron transitions from the valence band of p-type silicon to the metal.

Hole/electron generation and recombination through defects are represented by a Hall-Schockley-Read (HSR) single level model [8,9] which characterizes defects with neutral and single charge states. Carrier generation/recombination through a single defect level center [10] is given by:

$$R = C \frac{pn - n_i^2}{n+p+2n;\ \mathrm{Cosh}\left[q(\phi_t - \phi_i) / k\,T\right]}, \qquad (2\text{-}3)$$

where ϕ_t represents the trap potential and ϕ_i ; represents the intrinsic Fermi potential in silicon.

Calculations suggest that at the temperatures considered here (77° K-110° K) terms in Eqs.2-1 involving electrons in p-type silicon will have a negligible influence upon the results attained. For this reason such terms have been neglected and, thereby, these equations are reduced to the form

$$\text{a)} \quad \frac{d^2\psi}{dx^2} = \frac{q}{K\epsilon_o} (N_A - p)$$

$$\text{b)} \quad J_p = -qD_p \frac{dp}{dx} - q\mu_p \frac{d\psi}{dx} \qquad (2\text{-}4)$$

$$\text{c)} \quad \frac{djp}{dx} = \frac{dJ_n}{dx} = C$$

2.0 Electric Current Continuity

Many investigations of diode operation neglect the influence of electric current upon the electrostatic potential distribution. Such a

simplification is achieved by maintaining constant the electron and hole quasi-Fermi potentials. In the presence of a large ionized impurity atom density little error results from this simplification, particularly when the reverse current is relatively small. Nonetheless, velocity limited carrier transport in a reverse biased diode does produce a significant amount of mobile carrier accumulation and, thereby, can modify the space-charge layer potential distribution.

For purposes of this analysis we attain electric current continuity by relating the divergence of electric current to the density of mobile carriers at a given location:

$$\frac{dJ_p}{dx} = R(p). \qquad (2\text{-}5)$$

Both drift and diffusion mechanisms are assumed to contribute to the total electric current in Eq.2-5 thus:

$$J_p = -qD_p \frac{dp}{dx} - q\mu_p p \frac{dp}{dx} . \qquad (2\text{-}6)$$

3.0 Temperature Dependent Parameters

At low temperatures (77° K-110° K) many physical and electrical properties of silicon differ from that realized at room temperature. Unfortunately, substantial work remains to accurately characterize silicon at low temperature but, nonetheless, it is believed that many important low temperature material parameters are available in the technical literature.

a) Energy Gap

The energy gap Eg in silicon can be shown slightly temperature dependent[11], and approximated by the relation:

$$Eg = 1.21 - 7.242\times10^{-3}\,(T/300) - 3.664\times10^{-2}(T/300)^2 \qquad (2\text{-}7)$$

This expression represents an empirical fit to Fig.2-10 of Ref.11.

b) Intrinsic Fermi-Level

The intrinsic Fermi-level E_i is usually assumed located at the mid-gap of silicon. Nonetheless, in more rigorous calculations the intrinsic Fermi-level deviates slightly from this midgap position:

$$E_i - Ev = Eg/2 + (k\ T/q)\ \ln\ (N_v/N_c)$$

$$= Eg/2 - 1.206 \times 10^{-2}(T/300), \qquad (2\text{-}8)$$

where Nv and Nc represent the effective density of states at the valence and conduction band edges, respectively. In Eq.2-8 we assume $(N_v/N_c) = 1.02/2.8$, as stated in Ref.11, p.359.

c) Intrinsic Carrier Density

The intrinsic carrier density in silicon is exceedingly dependent upon the temperature, as shown in Ref.12, p.27:

$$n_i^2 = 4.9 \times 10^{15}(M_h^* M_e / M^2)^{3/4}\ T^{3/2}\ \exp(-E_g / 2\ k\ T) \qquad (2\text{-}9)$$

where M_h^* and M_e^* are the density of states effective mass for holes and electrons, respectively, and M is the free electron mass. This expression is approximated by

$$n_i = 3.925 \times 10^{19}(T/300)^{3/2}\ \exp\ (-\ E_g/2\ k\ T) \qquad (2\text{-}10)$$

In Eq.2-10 the leading constants have been adjusted so that n_i equals $1.5 \times 10^{10}/cm^3$ when $T = 300°\ K$.

d) Bulk Hole Density

In charge-neutral regions of p-type silicon the hole density is given by

$$p = n_i \exp\ (E_i - E_f) / k\ T \qquad (2\text{-}11)$$

where n_i represents the intrinsic carrier density, E_i is the intrinsic Fermi-level, and E_f is the Fermi-level. Clearly, the hole density in charge neutral p-type silicon is exceedingly dependent upon the temperature.

e) Ionized Acceptor Density

The ionized acceptor density can be calculated using an expression of the form[13]:

$$N_I = \frac{N_A}{1 + \left[4 + 2\ \exp\ (-q\Delta/k\ T)\right]\ \exp\ \left[-q(E_A - E_F) / k\ T\right]} \qquad (2\text{-}12)$$

where Δ = .044 ev; this term accounts for the spin orbit splitting at the valence band maximum in silicon.

f) Fermi-Level

Calculation of the Fermi-level E_F at a given temperature represents an iterative process. Specifically, at any given temperature T the Fermi-level must be such that charge neutrality exists in the material under consideration:

$$-N_A + p - n = 0. \qquad (2\text{-}13)$$

In this calculation we ignore the electron density since at low temperatures this term has negligible influence upon Eq.2-13. Substituting Eq.2-10 into Eq.2-11 yields the hole

density in terms of the Fermi-level E_F. Thereafter, we substitute this expression and Eq.2-12 into Eq.2-13. We have the electrostatic charge in intrinsic silicon, as a function of the Fermi-level E_F. Thereafter the Fermi-level can be established using iterative methods to produce an electrostatic charge of zero.

Although the low-temperature mobility for holes is available in the technical literature[13], to date, this has not been implemented into this mathematical model.

4.0 Finite-Difference Implementation

Using traditional finite-difference techniques, this problem is solved on a one-dimensional grid containing a specified number of points (MAX = 100). These points are assumed equally spaced, and located between the ohmic contact to p-type silicon, and the metal-semiconductor interface.

In one spatial dimension, we designate a unit-cell of this one-dimensional array as composed of three locations: left, right, and center. Thereafter, applying central difference techniques in conjunction with the Taylor series, we can express the second derivative of electrostatic potential at this center location by the relation:

$$\left.\frac{d^2\psi}{dx^2}\right|_c \approx \frac{\psi_l - 2\psi_c + \psi_r}{\Delta x^2}, \qquad (2\text{-}14)$$

where Δx represents the distance between points on this array. Thereby, Poisson's equation in finite-difference form is given by

$$\frac{\psi_l - 2\psi_c + \psi_w}{\Delta x^2} = Q_c, \qquad (2\text{-}15)$$

where Q_c is the electrostatic charge and is given by:

$$Q_c = \frac{q}{\kappa \epsilon_o} (N_A - p). \tag{2-16}$$

An equation similar to Eq. 2-16 can be written for each point on our approximating grid. When this is done we have 100 points and 100 equations, with 100 unknowns---the electrostatic potential at each location of the approximating grid.

Such a system of equations can be written in matrix form yielding a tri-diagonal matrix of rank 100. There is a multitude of different ways one can solve this matrix problem, each method yielding particular advantages and disadvantages.

A particular source of difficulty in finite-difference analysis is round-off error when solving large systems of equations. For this reason we have adopted the choleski decomposition technique[14-16], which has been found exceedingly stable in the presence of round-off error.

The choleski technique is based upon the fact that if a matrix B is positive definite, than B can be written as the product of a lower triangular matrix L and its transpose L^t thus

$$B = LL^t \tag{2-17}$$

and we have a two-step solution for this matrix problem.

It is emphasized that despite a direct solution for this matrix problem, solving Poisson's equation remains an iterative process. The exact mobile hole distribution is unknown and, therefore, iteration between the solution for $\psi(x)$ and $p(x)$ must continue until convergence is attained.

In an attempt to accelerate convergence of Poisson's equation we make use of Gummels algorithm [17]. This algorithm is based upon a linear approximation of the exponential relations appearing in the Boltzmann equa-

tion for holes, Eq.2-2b. We assume ψ^m, and p^m represent values of electrostatic potential and holes respectively, from m^{th} iteration step. Further, let $\psi^{m+1} = \psi^m + \delta^{m+1}$ where δ^{m+1} represents a small quantity. Thus, from the Boltzmann relation

$$\exp(\psi^{m+1}) = \exp(\psi^m) \left[1 + \delta^{m+1} \right] \tag{2-18}$$

thus

$$p^{m+1} = n^m \ (1 - \delta^{m+1}) \tag{2-19}$$

representing a prediction for the hole density at any location, resulting from the next iteration. Thereby, using Poisson's equation we have:

$$\frac{d^2 \psi^{m+1}}{dx^2} - \frac{q}{\kappa \epsilon_o} (p^m) \psi^{m+1} = \frac{q}{\kappa \epsilon_o} \left[N_A - p^m - p^m \psi^m \right]. \tag{2-20}$$

In finite difference form only the center terms need be modified: one term added to the finite difference element and a second term to the charge element.

In calculations of electric current continuity it is customary to employ similar finite-difference approximations to the expression for electric current, Eq.2-6, and substitute the results into an expression for the divergence of electric current. However, it can be shown that this procedure leads to numerical instability whenever the voltage difference between two mesh points exceeds about 5.1×10^{-2} volts [18]. Following Sharfetter and Gummel, the expression for electric current,

$$J_p = - qD_p \frac{dp}{dx} - q \mu_p p \frac{d\psi}{dx} , \tag{2-21}$$

is treated as a differential equation in p with J_p, μ_p and $d\psi/dx$ assumed constant between mesh points.

Thereby, we have a differential equation of the form

$$\frac{dp}{dx} + Ap + B = 0 \qquad (2\text{-}22)$$

which can be solved between two finite-difference mesh points yielding

$$p_{n+1} = p_n \exp(U_{n+1} - U_n) - \frac{J\Delta x}{\mu (U_{n+1} - U_n)} \left[\exp(U_{n+1} - U_n) - 1\right] \qquad (2\text{-}23)$$

where U represents the normalized electrostatic potential ($U = q\psi / k T$). Equation (2-23) relates the hole density at mesh point n+1 and n to the electric current between these mesh points. From Eq.(2-23) we can therefore write

$$J = \mu \frac{p_n \mu \Delta U}{\Delta x \left[\exp(\Delta U) - 1\right]} + \frac{p \mu \Delta U}{\Delta x \left[\exp(-\Delta U) - 1\right]} \qquad (2\text{-}24)$$

where $\Delta U = U_{n+1} - U_n$. Equation (2-24) expresses the electric current between mesh points n and n+1 in terms of the potential and hole densities at these locations.

Designating the electric current into node n by J_w and out of node n by J_e, the divergence of electric current at node n is given by:

$$\frac{dJ_n}{dx} \approx \frac{J_e - J_w}{\Delta x} = C_n$$

where C represents the recombination/generation term assigned to node n. After substituting Eq.2-24 into Eq.2-25 for the east and west electric currents we obtain an expression for the divergence of electric current at each node in terms of the hole density at this node, and the two adjacent nodes.

Thereby we obtain a system of equations for the hole density---one equation for each node. This system represents a matrix equation for electron density that contains a sparce, tri-diagonal matrix. This system of equations is solved using the technique of Gauss elimination; by reducing the matrix to a triangular form and, thereafter, solving for the electron densities through backward substitution.

5.0 Boundary Conditions

Boundary conditions for this calculation are introduced in two different arrays: first, in the electrostatic potential array and, second, in the hole density array. Recognizing that all essential potential drop within a Schottky barrier device is encountered within the semiconductor material, this situation is introduced through an adjustment of the boundary conditions. Additionally, this mathematical model is directed toward an effective generation of holes at the metal-semiconductor interface; such a mechanism is also introduced through an adjustment of boundary conditions at this location.

For the solution of Poisson's equation we assume both end points of the one-dimensional array are maintained at a specified electrostatic potential: zero at the barrier interface, and at some positive applied voltage at the semiconductor ohmic contact. At each of these locations we have a finite-difference equation of the type:

$$A\,\psi_w + B\,\psi_c + D\,\psi_e = Q_c \qquad (2\text{-}26)$$

If we designate the barrier interface at the western most location and the ohmic contact as the eastern most location, it is clear that A at the barrier and D at the ohmic contact do not, in fact, exist. Thus, setting

$$\text{(Barrier boundary)}\quad D = O,\ B = 1,\ Q_c = (-N_A + p)$$

$$\text{(ohmic contact)}\quad A = O,\ B = 1,\ Q_c = V_{appl}$$

The boundary conditions for the potential array are readily satisfied.

In the presence of an electric current the hole quasi-Fermi potential has some unspecified gradient distribution between the ohmic contact and the barrier interface. This gradient distribution is unknown, and it will depend upon the electric current density at each location within the device. If, indeed, the semiconductor ohmic contact lies far removed from the diode space-charge layer, the quasi-Fermi potential at that location will equal Fermi-potential, and at a point that is charge neutral. Further, if the hole Fermi-potential is maintained constant from the ohmic contact to the Schottky barrier we would model a device of this type in the absence of an electric current. Thus, reasonable boundary conditions appear to be attained by maintaining at the ohmic contact a hole quasi-Fermi potential equal to the Fermi-potential for the p-type semiconductor material. At the barrier interface we calculate the hole density using Eq.1-18, and thereby establish the quasi-Fermi potential at that location.

Thus, with knowledge of the quasi-Fermi potentials at the ohmic contact and at the barrier interface we can readily calculate the electron densities at these locations and, thereby, establish boundary conditions for solving the equation of electric current continuity.

6.0 Iterative Solution for the Schottky Barrier Diode

As previously discussed, iterative techniques are used to solve this problem of the Schottky barrier diode. A given solution is initiated by a first "guess" concerning the electrostatic potential and the hole density distributions. Thereafter, using iterative techniques, Poisson's equation is solved, and after each solution the hole distribution is updated, maintaining the initial guess for the hole quasi-Fermi potential; by recalculating the hole density we are establishing an improved solution for the electrostatic charge distribution.

Prior to each new calculation of the electrostatic charge in Poisson's equation, a determination is made concerning the degree of convergence. This is accomplished by calculating for each location of the potential array the expression:

$$A\,\psi_e + B\,\psi_c + D\,\psi_w - Q_c = R \qquad (2\text{-}27)$$

which yields the error, or residual, at a given spatial location. Ideally, the true solution for this problem would yield a residual of zero everywhere.

Termination of this particular aspect of the calculation is attained when the maximum residual upon entry to the potential calculation is 10^{-4} (or less). Experience shows that any attempt at further refining the solution is of little practical value. In practice, this initial convergence of Poisson's equation is obtained with 100 (or less) iterations between electrostatic potential calculation and the hole density, for a given quasi-Fermi potential calculation.

After attaining convergence for this initial part of the potential calculation we obtain a very accurate solution for Poisson's equation, for our first guess about the quasi-Fermi potential distribution. Next, an improved solution for the quasi-Fermi potential is attained by solving the continuity equation for the hole density and recalculating a new quasi-Fermi potential.

After the initial convergence of Poisson's equation we no longer require the iteration between the electrostatic potential calculation and the hole density, maintaining the quasi-Fermi potential constant. After each new solution of Poisson's equation we immediately recalculate a new hole distribution and, hence, a new hole quasi-Fermi potential.

Final convergence for this sytem of equations is based upon simultaneously attaining three differnt convergence criterion:

1. When the starting residual is low prior to entry into the electrostatic potential calculation.

2. When the starting residual is low prior to entry into the calculation of electric current continuity.

3. When electric current continuity is attained within 1% of the total electric current.

From a practical point of view, excellent convergence is usually attained within 100 iterations between the solution of Poisson's equation and the solution for electric current continuity.

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APPENDIX 1

Computer Programs Developed During This Investigation

Note: All computer programs listed in APPENDIX 1 are self contained. The listings within a given function group can be keypunched, compiled, linked, and run as a unit.

APPENDIX 1-A

Program for Calculating the Fermi-Level vs. Temperature

```
      COMPILER DOUBLE PRECISION
C
C     ================================================================
C
C     MAIN PROGRAM FOR CALCULATING THE FERMI LEVEL IN A CONDUCTOR
C     CONTAINING A SPECIFIED FREE ELECTRON DENSITY
C
C
C     USEAGE:REQUIRES THE FOLLOWING SUBPROGRAMS:
C            FUNCTION EFERMI
C            SUBROUTINE ROOT
C            FUNCTION QUAD1
C            FUNCTION XINT
C
C            TEXP=EXPONENT FOR TEMP.
C            JMAX=TOTAL NUMBER OF ELECTRON DENSITY STEPS
C            EDLT=ELECTRON DENSITY STEP SIZE
C            EEXP=EXPONENT FOR ELECTRON DENSITY
C            KMAX=TOTAL NUMBER OF TEMP STEPS
C            TDLT=TEMP STEP SIZE
C            EMASS=ELECTRON MASS RATIO (M*/M)
C
C            LUOUT=CHANNEL FOR OUTPUT
C
C     ================================================================
C
C     ORIGIONAL: D.P. KENNEDY & ASSOC. GAINESVILLE FLA.
C
C     ================================================================
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL EFERMI
C
C     -----INITIALIZE MISC CONSTANTS-----
C
      EDLT=1.0D0
      EEXP=2.0D1
      KMAX=4
      EMASS=1.0D0
      TEXP=-2.5
      TDLT=1.0D-1
```

```
      JMAX=13
      LUOUT=10
C
C     -----TOP OF ELECTRON DENSITY STEPPING-----
C
      DO 20 K=1,KMAX
      ELECT=1.0D1**EEXP
C
C     -----TOP OF TEMP STEPPING LOOP-----
C
      XEXP=TEXP
      DO 10 J=1,JMAX
      T=1.0D1**(XEXP)
C
C     -----CALCULATE FERMI LEVEL AT ZERO K-----
C
      EF0=3.0D0*ELECT*1.0D-21/(EMASS**(3.0D0/2.0D0)*6.314)
      EF0=EF0**(2.0D0/3.0D0)
      EF0=EF0/(8.617D-5*T)
C
C     -----CALCULATE FERMI LEVEL-----
C
      DUMMY(1)=EF0
      EF=EF0*0.75D0
      EFMAX=1.0D2*EF0
      DELTE=EF0*5.0D-1
      EPS=1.0D-4
C
      CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT,'ROOT NOT FOUND')
      IF(IER.NE.1) STOP
C
      WRITE(LUOUT,1111) TEXP,EF,EF0
 1111 FORMAT(1X,'TEXP=',1PD8.1,3X,'EF=',1PD11.4,3X,'EF0=',1PD11.4)
      XEXP=XEXP+TDLT
   10 CONTINUE
      END
```

```
C
C     ================================================================
C
C     FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
C                      METALLIC CONDUCTOR
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      FUNCTION EFERMI(EF,DUMMY)
      DIMENSION DUMMY(10)
      EXTERNAL XINT
C
C     -----INTEGRATE FROM 0 TO INF-----
C
      EF0=DUMMY(1)
      DUMMY(2)=EF
      SUM=0.0D0
      XX=EF-1.2D1
      IF(XX.GT.0.3D0) SUM=2.0I0*(XX**(3.0D0/2.0D0))/3.0D0
      XUBND=0.0D0
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      XLBND=XUBND
      XUBND=XUBND+1.0D1
      XX=XUBND-EF
      IF(XX.GT.1.0D2) GOTO 30
      CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   30 CONTINUE
      EFERMI=1.0D0-3.0D0*EF0**(-3.0D0/2.0D0)*SUM/2.0D0
C
C
```

```
RETURN
END
```

```
C
C
C     ==========================================================
C
C     SUBROUTINE "ROOT" : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
C
C     USAGE  :   CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     WHERE  :   B(X,DUMMY)  =  ARBITRARY FUNCTION
C
C     .          DUMMY       =  A 10 ELEMENT ARRAY USED FOR PASSING
C     .                         PARAMETERS TO THE FUNCTION "B"
C
C     .          X           =  MIN (MAX) VALUE OF X BEGINING SEARCH
C
C     .          XMAX        =  MAX (MIN) VALUE OF X DURING SEARCH
C
C     .          DELX        =  INITIAL STEP SIZE
C     .                         ( +DELX INCREASES X . -DELX DECREASES X )
C
C     .          EPS         =  PERMITTED FRACTIONAL ERROR
C
C     .          IAR         =  ITERATION METHOD
C     .                         ( IAR = 0  BINARY CHOP )
C     .                         ( IAR = 1  METHOD OF SECANTS )
C
C     .          IER         =  ERROR FLAG
C     .                         ( IER = 1 ROOT FOUND )
C     .                         ( IER = 0 ROOT NOT FOUND )
C
C     COMMENT :  THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
C     .          PROGRAM MUST CLASSIFY THE FUNCTION NAME
C     .          TO BE PASSED THROUGH "B" AS EXTERNAL.
C
C     ==========================================================
C     ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
C
C     MOD#1    : AERC  C.L. KENNEDY   NOV. 1978
C     .                  IF X REACHES XMAX SET X=0 AND RETURN
C
```

```
C     MOD#C    : AERC  D.P. KENNEDY NOV 1978
C     .                    INTRODUCED ERROR FLAG IER
C
C     MOD#B    : AERC  D.P. KENNEDY  NOV. 1978
C     .                    EPS=FRACTIONAL CHANGE IN X
C     .                    METHOD OF SECANTS INTRODUCED
C
C     MOD#A    : AERC  C.L. KENNEDY  DECEMBER 1978
C     .                    ALL DUMMY VARIABLES PASSED
C     .                    THROUGH ARRAY DUMMY
C
C     ================================================================
C
      SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAP,IER,DUMMY)
C
      #      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION P(2),Q(2),DUMMY(1)
C
      IF (DELX.EQ.0.0D0) GOTO 90
      IER=1
      P(1)=0.0D0
      P(2)=0.0D0
      Q(1)=0.0D0
      Q(2)=0.0D0
      Y=B(X,DUMMY)
      P(1)=X
C
C     ----------------------------------------------------------------
C     S T E P   T O   B R A C K E T   R O O T
C     ----------------------------------------------------------------
C
   10 X=X+DELX
      P(2)=X
      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
```

```
      IF(A.LT.0.0D0) GOTO 15
      Y=Z
      GOTO 10
C
C     ------------------------------------------------------------
C     B I N A R Y  C H O P  O R  M E T H O D  O F  S E C A N T S ?
C     ------------------------------------------------------------
C
   15 DEL=DELX
      IF(IAR.EQ.1) GOTO 60
C
C     ------------------------------------------------------------
C     B I N A R Y   C H O P
C     ------------------------------------------------------------
C
   20 Y=Z
      P(1)=P(2)
   30 DEL=DEL/2.0D0
      X=X-DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 40
      GOTO 30
C
   40 Y=Z
      P(1)=P(2)
   50 DEL=DEL/2.0D0
      X=X+DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 20
      GOTO 50
C
C     ------------------------------------------------------------
```

```
C     M E T H O D   O F   S E C A N T S
C     ---------------------------------------------------------------
C
   60 Q(2)=Z
      P(2)=X
      P(1)=X-DEL
      PREP=P(1)
      Q(1)=B(DUMMY,PREP)
   70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
      YY=B(XX,DUMMY)
      P(1)=P(2)
      Q(1)=Q(2)
      P(2)=XX
      Q(2)=YY
      ERROR=DABS((P(1)-P(2))/P(2))
      IF(ERROR.LE.EPS) GOTO 80
      GOTO 70
   80 X=XX
      RETURN
C
C     ---------------------------------------------------------------
C     E R R O R   R E T U R N   X = 0   I E R = 0
C     ---------------------------------------------------------------
C
   90 X=0.0D0
      IER=0
      RETURN
      END
```

```
C     ================================================================
C     SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
C                       LEGENDRE TYPE
C
C
C     USEAGE: CALL QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C             FUNC   =FUNCTION TO BE INTEGRATED. THIS FUNCTION
C                     MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
C             DUMMY  = 1-DIM DUMMY ARRAY FOR PASSING DATA
C                      TO FUNC. THIS ARRAY MUST BE DIMENTIONED
C                      IN THE CALLING PROGRAM.
C .           XLBND  = LOWER BOUND OF THE INTEGRAL
C .           XUBND  = UPPER BOUND OF THE INTEGRAL
C .           RES    = RESULT
C             IAR    = NUMBER OF TERMS IN THE INTEGRATION
C                      (MAX=16,MIN=2)
C
C
C       NOTE:
C .          FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
C .               CALLING PROGRAM
C
C
C     REFERENCE:
C .          NUMERICAL ANALYSIS. Z.KOPAL, CHAPTER VII,
C .               CHAPMAN HALL, LONDON, 1961
C
C
C     ================================================================
C     ORIGIONAL:C.L. KENNEDY OCT. 1978
C                  C.L. KENNEDY
C       MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
C             TO 16 TERMS  SEPT 1981
C     ================================================================
C
C
      SUBROUTINE QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C
C
      COMMON /QUAD/ Z(8,16),W(8,16)
```

```
      DIMENSION DUMMY(1)
C
      DATA Z / 8*0.0D0,
     $.5773502691896265D0,7*0.0D0,
     $0.7745966692414834D0,7*0.0D0,
     $0.8611363115940526D0,0.3399810435848563D0,6*0.0D0,
     $0.9061798459386644D0,0.5384693101056831D0,6*0.0D0,
     $0.9324695142031521D0,0.6612093864662645D0,0.2386191860831969D0,5*0.0D0,
     $0.9491079123427585D0,0.7415311855993945D0,0.4058451513773972D0,5*0.0D0,
     $0.9602898564975362D0,0.7966664774136267D0,0.5255324099163290D0,
     $0.1834346424956498D0,4*0.0D0,
     $0.9681602395076261D0,0.8360311073266358D0,0.6133714327005904D0,
     $0.3242534234038089D0,4*0.0D0,
     $0.9739065285171717D0,0.8650633666889845D0,0.6794095682990244D0,
     $0.4333953941292471D0,0.1488743389816312D0,3*0.0D0,
     $0.9782286581460570D0,0.8870625997680950D0,0.7301520055748049D0,
     $0.5190961292068129D0,0.2695431559523450D0,3*0.0D0,
     $0.9815606342467190D0,0.9041172563704750D0,0.7699026741943050D0,
     $0.5873179542866130D0,0.3678314989981800D0,0.1252334085114690D0,
     $2*0.0D0,
     $0.9841830547185880D0,0.9175983992229780D0,0.8015780907333100D0,
     $0.6423493394403400D0,0.4484927510364470D0,0.2304583159551350D0,
     $2*0.0D0,
     $0.9862838086968120D0,0.9284348836635740D0,0.8272013150697650D0,
     $0.6872929048116850D0,0.5152486363581540D0,0.3191123689278900D0,
     $0.1080549487073440D0,0.0D0,
     $0.9879925180204850D0,0.9372733924007060D0,0.8482065834104270D0,
     $0.7244177313601700D0,0.5709721726085390D0,0.3941513478077560D0,
     $0.2011940939974350D0,0.0D0,
     $0.9894009349916500D0,0.9445750230732330D0,0.8656312023878320D0,
     $0.7554044083550030D0,0.6178762444026440D0,0.4580167777657220D0,
     $0.2816035507792590D0,0.0950125098376370D0/
C
      DATA W / 8*0.0D0,
     $1.0D0,7*0.0D0,
     $0.5555555555555560D0,0.8888888888888890D0,6*0.0D0,
     $0.3478548451374540D0,0.6521451548625460D0,6*0.0D0,
     $0.2369268850561890D0,0.4786286704993660D0,0.5688888888888890D0,
     $5*0.0D0,0.1713244923791700D0,0.3607615730481390D0,
     $0.4679139345726910D0,5*0.0D0,0.1294849661688700D0,
     $0.2797053914892770D0,0.3818300505051190D0,0.4179591836734690D0,
     $4*0.0D0,0.1012285629037600D0,0.2223810344533740D0,
```

```
     $Ø.313706645877887DØ,Ø.362683783378362DØ,
     $4*Ø.ØDØ,Ø.Ø8127438836157 4DØ,Ø.183648162694257DØ,
     $Ø.262610696402935DØ,Ø.312347077040223DØ,Ø.330239355001260DØ,
     $3*Ø.ØDØ,Ø.066671344308688DØ,Ø.149451349150581DØ,
     $Ø.219086362515982DØ,Ø.269266719309996DØ,Ø.295524224714753DØ,
     $3*Ø.ØDØ,Ø.055668567116174DØ,Ø.125580369464905DØ,
     $Ø.186290210927734DØ,Ø.233193764591990DØ,
     $Ø.262804544510247DØ,Ø.272925086777901DØ,2*Ø.ØDØ,
     $Ø.047175336386512DØ,Ø.106939325995318DØ,Ø.160078328543346DØ,
     $Ø.203167426723066DØ,Ø.233492536538355DØ,Ø.249147045813403DØ,
     $2*Ø.ØDØ,Ø.040484004765316DØ,Ø.092121499837728DØ,
     $Ø.138873510219787DØ,Ø.178145980761946DØ,Ø.207816047536889DØ,
     $Ø.226283180262897DØ,Ø.232551553230874DØ,Ø.ØDØ,
     $Ø.035119460331752DØ,Ø.080158087159760DØ,Ø.121518570687903DØ,
     $Ø.157203167158194DØ,Ø.185538397477938DØ,Ø.205198463721296DØ,
     $Ø.215263853463158DØ,Ø.ØDØ,Ø.030753241996117DØ,
     $Ø.070366047488108DØ,Ø.107159220467172DØ,Ø.139570677926154DØ,
     $Ø.166269205816994DØ,Ø.186161000015562DØ,Ø.198431485327112DØ,
     $Ø.202578241925561DØ,Ø.027152459411754DØ,Ø.062253523938648DØ,
     $Ø.095158511682493DØ,Ø.124628971255534DØ,Ø.149595988816577DØ,
     $Ø.169156519395003DØ,Ø.182603415044924DØ,Ø.189450610455068DØ/
C
      SUM=Ø.ØDØ
      DO 1Ø I=1,8
      IF(W(I,IAR).EQ.Ø) GOTO 1Ø
      ARG=(Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.ØDØ
      TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
      ARG=(-Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.ØDØ
      TERM2=Ø.ØDØ
      IF(Z(I,IAR).NE.Ø.ØDØ) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
      SUM=SUM+TERM1+TERM2
   1Ø CONTINUE
C
      RES=SUM*(XUBND-XLBND)/2.ØDØ
C
      RETURN
      END
```

QUAD'.GV - 3

```
      FUNCTION XINT(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION XINT REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   OCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
C
      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      XINT=A/DENOM
C
C
      RETURN
      END
```

APPENDIX I-B

Program for Calculating Unoccupied Energy States Between the Conduction Band Edge E_c and the Fermi-Level E_f

```
      COMPILER DOUBLE PRECISION
C
C     ================================================================
C
C     MAIN PROGRAM FOR CALCULATING THE DENSITY OF UNOCCUPIED
C     ENERGY STATES THAT RESIDE BETWEEN THE CONDUCTION BAND
C     EDGE AND THE FERMI LEVEL
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1,FUNCTION DIST, SUBROUTINE ROOT
C              SUBROUTINE XFERMI,FUNCTION EFERMI,AND FUNCTION XINT
C
C              TEXP=EXPONENT FOR TEMP STEPPING
C              TDLT=TEMP STEP SIZE
C              JMAX=NUMBER OF TEMP STEPS
C              EEXP=EXPONENT FOR ELECT. DENSITY STEPPING
C              EDLT=ELECT. DENSITY STEP SIZE
C              KMAX=MAX NUMBER OF ELECT. DENSITY STEPS
C              EMASS=ELECTRON MASS RATIO (M*/M)
C
C
C              LUOUT=CHANNEL FOR OUTPUT
C
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EXTERNAL DIST
C
C
C
C     -----INITIALIZE MISC CONSTANTS-----
C
      TEXP=-2.5
      TDLT=1.0D-1
      JMAX=13
```

```
      EEXP=2.3D1
      EOLT=1.0D0
      KMAX=4
      EMASS=1.0D0
      LUOUT=13
C
C     -----TOP OF ELECTRON DENSITY STEPPING LOOP-----
C
      DO 40 K=1,KMAX
      ELECT=1.0D1**EEXP
C
C     -----TOP OF TEMP STEPPING LOOP-----
C
      XEXP=TEXP
      DO 30 J=1,JMAX
      T=1.0D1**(-XEXP)
C
C     -----CALCULATE FERMI LEVEL-----
C
      CALL XFERMI(ELECT,EF0,T,EMASS,EF,LUOUT)
C
C     -----INTEGRATE FROM EC TO EF-----
C
      IEXIT=0
      SUM=0.0D0
      XUBND=0.0D0
   25 CONTINUE
      IF(IEXIT.EQ.1) GOTO 27
      XLBND=XUBND
      XUBND=XUBND+1.0D-2
      IF(EF.GT.5.0D2) XUBND=XUBND+1.0D-3
      IF(XUBND.GT.1.0D0) IEXIT=1
      IF(IEXIT.EQ.1) XUBND=1.0D0
      DUMMY(1)=EF
      CALL QUAD1(DIST,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 25
C
   27 CONTINUE
      XX=-3.0D0/2.0D0
      ANS=3.0D0*((EF0/EF)**(XX))*SUM/2.0D0
C
```

```
      WRITE(LUOUT) ANS=',ANS
      A(J)=DLOG10(ANS)
      P(J)=XEXP
      XEXP=XEXP*0.150
   30 CONTINUE
      EEXP=EEXP+EDLT
   40 CONTINUE
      END
```

100

FIG2.0V - 3

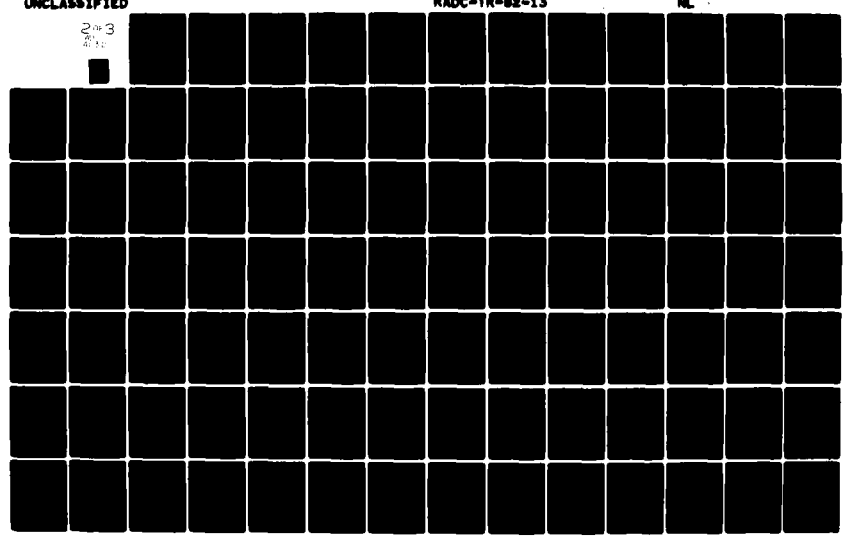
```
      COMPILER DOUBLE PRECISION
C
C     ================================================================
C
C     SUBROUTINE XFERMI IS USED TO CALCULATE  THE FERMI LEVEL
C                     IN A METAL AT A SPECIFIED TEMP
C
C     USEAGE: REQUIRES THE FOLLOWING
C             FUNCTION EFERMI
C             SUBROUTINE ROOT
C             FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.
C
C     ================================================================
C
      SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUOUT)
C
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL EFERMI
C
C
C
C     -----CALCULATE FERMI LEVEL AT ZERO K-----
C
      EF0=3.0D0*ELECT*1.0D-21/(EMASS**(3.0D0/2.0D0)*1.2360D1)
      EF0=EF0**(2.0D0/3.0D0)
      EF0=EF0/(8.617D-5*T)
C
C     -----CALCULATE FERMI LEVEL-----
C
      DUMMY(1)=EF0
      EF=EF0*0.75D0
      EFMAX=1.0D2*EF0
      DELTE=EF0*5.0D-1
      EPS=1.0D-4
C
```

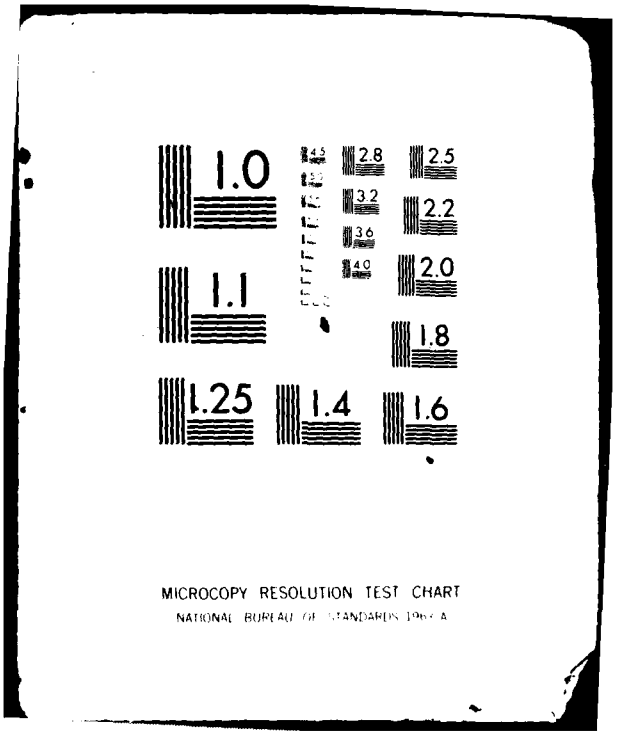
```
CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
IF(IER.NE.1) WRITE(LUOUT) 'ROOT NOT FOUND'
IF(IER.NE.1) STOP
END
```

```
C     ==========================================================
C
C     FUNCTION EFERMI IS USED TO CALC. THE FERMI LEVEL IN A
C                     METALLIC CONDUCTOR
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
C
C     ==========================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ==========================================================
C
      FUNCTION EFERMI(EF,DUMMY)
      DIMENSION DUMMY(10)
      EXTERNAL XINT
C
C     -----INTEGRATE FROM 0 TO INF-----
C
      EF0=DUMMY(1)
      DUMMY(2)=EF
      SUM=0.0D0
      XX=EF-1.2D1
      IF(XX.GT.0.0D0) SUM=2.0D0*XX**(3.0D0/2.0D0)/3.0D0
      XUBND=0.0D0
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      XLBND=XUBND
      XUBND=XUBND+1.0D1
      XX=XUBND-EF
      IF(XX.GT.1.0D2) GOTO 30
      CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   30 CONTINUE
      EFERMI=1.0D0-3.0D0*EF0**(-3.0D0/2.0D0)*SUM/2.0D0
C
C
```

AD-A113 211 KENNEDY (D P) AND ASSOCIATES INC GAINESVILLE FL F/G 20/12
INVESTIGATION OF THE CURRENT VOLTAGE RELATIONSHIP FOR LOW BARRI--ETC(U)
FEB 82 D P KENNEDY F19628-80-C-0020

UNCLASSIFIED RADC-TR-82-13 NL




1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS 1963 A

```
      RETURN
      END
```

```
C
C
C     ================================================================
C
C     SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
C
C     USAGE  :   CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     WHERE  :   B(X,DUMMY)  =  ARBITRARY FUNCTION
C
C     .          DUMMY       =  A 10 ELEMENT ARRAY USED FOR PASSING
C     .                         PARAMETERS TO THE FUNCTION "B"
C
C     .          X           =  MIN (MAX) VALUE OF X BEGINING SEARCH
C
C     .          XMAX        =  MAX (MIN) VALUE OF X DURING SEARCH
C
C     .          DELX        =  INITIAL STEP SIZE
C     .                         ( +DELX INCREASES X , -DELX DECREASES X )
C
C     .          EPS         =  PERMITTED FRACTIONAL ERROR
C
C     .          IAR         =  ITERATION METHOD
C     .                         ( IAR = 0  BINARY CHOP )
C     .                         ( IAR = 1  METHOD OF SECANTS )
C
C     .          IER         =  ERROR FLAG
C     .                         ( IER = 1 ROOT FOUND )
C     .                         ( IER = 0 ROOT NOT FOUND )
C
C     COMMENT :  THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
C     .          PROGRAM MUST CLASSIFY THE FUNCTION NAME
C     .          TO BE PASSED THROUGH "B" AS EXTERNAL.
C
C     ================================================================
C     ORIGINAL : APPLIED ELECTRONIC RESEARCH. GAINESVILLE. FLA. DEC. 1977
C
C     MOD#1    : AERC  C.L. KENNEDY   NOV. 1978
C     .                  IF X REACHES XMAX SET X=0 AND RETURN
C
```

```
C     MOD#2    : AERO  I.P. KENNEDY NOV 1978
C     .                INTRODUCED ERROR FLAG IER
C
C     MOD#3    : AERO  D.P. KENNEDY  NOV. 1978
C     .                EPS=FRACTIONAL CHANGE IN X
C     .                METHOD OF SECANTS INTRODUCED
C
C     MOD#4    : AERO  C.L. KENNEDY DECEMBER 1978
C     .                ALL DUMMY VARIABLES PASSED
C     .                THROUGH ARRAY DUMMY
C
C     ================================================================
C
C
      SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     #      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION P(2),Q(2),DUMMY(1)
C
      IF (DELX.EQ.0.0D0) GOTO 90
      IER=1
      P(1)=0.0D0
      P(2)=0.0D0
      Q(1)=0.0D0
      Q(2)=0.0D0
      Y=B(X,DUMMY)
      P(1)=X
C
C     ----------------------------------------------------------------
C     S T E P    T O    B R A C K E T    R O O T
C     ----------------------------------------------------------------
C
   10 X=X+DELX
      P(2)=X
      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
```

```
      IF(A.LT.0.0D0) GOTO 15
      Y=Z
      GOTO 10
C
C     ------------------------------------------------------------------
C     B I N A R Y   C H O P   O R   M E T H O D   O F   S E C A N T S  ?
C     ------------------------------------------------------------------
C
   15 DEL=DELX
      IF(IAR.EQ.1) GOTO 60
C
C     ------------------------------------------------------------------
C     B I N A R Y   C H O P ?
C     ------------------------------------------------------------------
C
   20 Y=Z
      P(1)=P(2)
   30 DEL=DEL/2.0D0
      X=X-DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 40
      GOTO 30
C
   40 Y=Z
      P(1)=P(2)
   50 DEL=DEL/2.0D0
      X=X+DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 20
      GOTO 50
C
C     ------------------------------------------------------------------
```

```
C     M E T H O D   O F   S E C A N T S
C     ---------------------------------------- ------- ----------

   60 Q(2)=Z
      P(2)=X
      P(1)=X-DEL
      PREP=P(1)
      Q(1)=B(DUMMY,PREP)
   70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
      YY=B(XX,DUMMY)
      P(1)=P(2)
      Q(1)=Q(2)
      P(2)=XX
      Q(2)=YY
      ERROR=DABS((P(1)-P(2))/P(2 )
      IF(ERROR.LE.EPS) GOTO 80
      GOTO 70
   80 X=XX
      RETURN
C
C     ------------------------------------------------------------
C     E R R O R   R E T U R N   X = 0   I E R = 0
C     ------------------------------------------------------------
C
   90 X=0.0D0
      IER=0
      RETURN
      END
```

```
      FUNCTION XINT(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION XINT:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   OCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(12)
      EF=DUMMY(2)
C
      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      XINT=A/DENOM
C
C
      RETURN
      END
```

```
C     ================================================================
C     SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
C                       LEGENDRE TYPE
C
C
C     USEAGE: CALL QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C             FUNC   =FUNCTION TO BE INTEGRATED. THIS FUNCTION
C                     MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
C             DUMMY  = 1-DIM DUMMY ARRAY FOR PASSING DATA
C                      TO FUNC. THIS ARRAY MUST BE DIMENTIONED
C                      IN THE CALLING PROGRAM.
C .           XLBND  = LOWER BOUND OF THE INTEGRAL
C .           XUBND  = UPPER BOUND OF THE INTEGRAL
C .           RES    = RESULT
C             IAR    = NUMBER OF TERMS IN THE INTEGRATION
C                      (MAX=16,MIN=2)
C
C
C       NOTE:
C .         FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
C .             CALLING PROGRAM
C
C
C     REFERENCE:
C .         NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
C .             CHAPMAN HALL, LONDON, 1961
C
C
C     ================================================================
C     ORIGIONAL:C.L. KENNEDY OCT. 1978
C               C.L. KENNEDY
C       MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
C             TO 16 TERMS  SEPT 1981
C     ================================================================
C
C
      SUBROUTINE QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C
C
      COMMON /QUAD/ Z(8,16),W(8,16)
```

```
      DIMENSION DUMMY(1)

      DATA Z / 8*0.0D0,
     $.5773502691896260D0,7*0.0D0,
     $0.7745966692414834D0,7*0.0D0,
     $0.8611363115940536D0,2.3399810435848566D0,6*0.0D0,
     $0.9061798459386640D0,0.5384693101056830D0,6*0.0D0,
     $0.9324695142031520D0,0.6612093864662650D0,0.2386191860831969D0,5*0.0D0,
     $0.9491079123427585D0,0.7415311855993940D0,0.4058451513773972D0,5*0.0D0,
     $0.9602898564975362D0,0.7966664774136267D0,0.5255324099163290D0,
     $0.1834346424956500D0,4*0.0D0,
     $0.9681602395076260D0,0.8360311073266360D0,0.6133714327005904D0,
     $0.3242534234038089D0,4*0.0D0,
     $0.9739065285171717D0,0.8650633666889850D0,0.6794095682990244D0,
     $0.4333953941292477D0,0.1488743389816310D0,3*0.0D0,
     $0.9782286581460570D0,0.8870625997680950D0,0.7301520055740490D0,
     $0.5190961292068120D0,0.2695431559523450D0,3*0.0D0,
     $0.9815606342467190D0,0.9041172563704750D0,0.7699026741943050D0,
     $0.5873179542866170D0,0.3678314989981800D0,0.1252334085114690D0,
     $2*0.0D0,
     $0.9841830547185880D0,0.9175983992229780D0,0.8015780907333100D0,
     $0.6423493394403410D0,0.4484927510364470D0,0.2304583159551350D0,
     $2*0.0D0,
     $0.9862838086968120D0,0.9284348836635740D0,0.8272013150697650D0,
     $0.6872929048116850D0,0.5152486363581540D0,0.3191123689278900D0,
     $0.1080549487073440D0,0.0D0,
     $0.9879925180204850D0,0.9372733924007060D0,0.8482065834104270D0,
     $0.7244177313601700D0,0.5709721726085390D0,0.3941513470775630D0,
     $0.2011940939974350D0,0.0D0,
     $0.9894009349916500D0,0.9445750230732330D0,0.8656312027878320D0,
     $0.7554044083550030D0,0.6178762444026440D0,0.4580167776572270D0,
     $0.2816035507792590D0,0.0950125098376370D0/

      DATA W / 8*0.0D0,
     $1.0D0,7*0.0D0,
     $0.5555555555555560D0,0.8888888888888890D0,6*0.0D0,
     $0.3478548451374540D0,0.6521451548625460D0,6*0.0D0,
     $0.2369268850561890D0,0.4786286704993660D0,0.5688888888888890D0,
     $5*0.0D0,0.1713244923791700D0,0.3607615730481390D0,
     $0.4679139345726910D0,5*0.0D0,0.1294849661688700D0,
     $0.2797053914892770D0,0.3818300505051190D0,0.4179591836734690D0,
     $4*0.0D0,0.1012285629037600D0,0.2223810344533740D0,
```

```
     $0.3137066458777887D0,0.3626887933783163D0,
     $4*0.0D0,0.08127438836157460,0.'80648'e3c9485770,
     $0.2606106964029350D0,0.3'234707704200230,0.330239395001
     $3*0.0D0,0.0666713443086880,0.1494513491505810,
     $0.2190863625159820,0.2692667193099960,0.29552402
     $3*0.0D0,0.0556685671'617480,0.1255803e9'649650,
     $0.1862902'892773400,0.2331937645919900,
     $0.2628045445102470,0.2729258867779'0'20.2*0.0D0,
     $0.0471753363865120,0.1869393599531800,0.1630078326543346D0,
     $0.2031674267230660,0.2334925365383551D0,0.249147045813403D0,
     $2*0.0D0,0.0434840047653160,0.0921214998377280,
     $0.1388735102197870,0.1781459807619460,0.207816047536389D0,
     $0.2262831802628970,0.2325515532308740,0.0D0,
     $0.0351194603317520,0.0801580871597600,0.1215185768790300,
     $0.1572031671581940,0.1855383974779380,0.2051984637212960,
     $0.2152638534631580,0.0D0,0.2387532419961170,
     $0.0703660474881080,0.1071592204671720,0.1395706792615400,
     $0.1662692058169940,0.1861610000155620,0.1984314853271120,
     $0.2025782419255610,0.0271524594117540,0.0622535239396480,
     $0.0951585116824930,0.1246289712555340,0.1495959888165770,
     $0.1691565193950030,0.1826034150449240,0.1894506104558680/
C
C
C
      SUM=0.0D0
      DO 10 I=1,8
      IF(W(I,IAR).EQ.0) GOTO 10
      ARG=(Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
      ARG=(-Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM2=0.0D0
      IF(Z(I,IAR).NE.0.0D0) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
      SUM=SUM+TERM1+TERM2
   10 CONTINUE
C
      RES=SUM*(XUBND-XLBND)/2.0D0
C
      RETURN
      END
```

```
      FUNCTION DIST(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   UNOCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EFC=DUMMY(1)
C
      A=DSQRT(ARG)
      B=EFC*(1.0D0-ARG)
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      DIST=A/DENOM
C
C
      RETURN
      END
```

APPENDIX 1-C

Program for Calculating Unoccupied Energy States Between the Fermi-Level E_f and an Energy E_b Where ($E_c < E_b < E_f$)

```
C
C     ================================================================
C
C     MAIN PROGRAM FOR CALCULATING THE DENSITY OF UNOCCUPIED
C     ENERGY STATES THAT RESIDE BETWEEN THE FERMY LEVEL AND
C     AN ARBITRARY ENERGY EB WHERE EC<EB<EF
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1,FUNCTION DIST, SUBROUTINE RDOT
C              SUBROUTINE XFERMI,FUNCTION EFERMI,AND FUNCTION XINT
C
C              TEXP=EXPONENT FOR TEMP STEPPING
C              TDLT=TEMP STEP SIZE
C              JMAX=NUMBER OF TEMP STEPS
C              RATIO=EB/EF RATIO
C              RDLT=STEP SIZE FOR RATIO
C              IMAX=MAX. NUMBER OF STEPS FOR RATIO
C              ELECT=FREE ELECTRON DENSITY
C              EMASS=ELECTRON MASS RATIO (M*/M)
C
C
C              LUOUT=CHANNEL FOR OUTPUT
C
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL DIST
C
C     -----INITIALIZE MISC CONSTANTS-----
C

      TEXP=-2.5
      TDLT=1.0D-1
      JMAX=13
      ELECT=1.0D20
      EMASS=1.0D0
```

```
      RATIO=0.1D0
      RDLT=1.0D-1
      IMAX=13
      LUOUT=10
C
C     -----TOP OF EB/EF STEPPING LOOP-----
C
      DO 40 I=1,IMAX
C
C     -----TOP OF TEMP STEPPING LOOP-----
C
      XEXP=TEXP
      DO 30 J=1,JMAX
      T=1.0D1**(-XEXP)
C
C     -----CALCULATE FERMI LEVEL-----
C
      CALL XFERMI(ELECT,EF0,T,EMASS,EF,LUOUT)
C
C     -----INTEGRATE FROM EB TO EF-----
C
      IEXIT=0
      SUM=0.0D0
      XUBND=1.0D0-1.2D1/EF
      IF(XUBND.LT.RATIO) XUBND=RATIO
   10 CONTINUE
      IF(IEXIT.EQ.1) GOTO 20
      XLBND=XUBND
      XUBND=XUBND+1.0D-2
      IF(EF.GT.5.0D2) XUBND=XUBND+1.0D-1
      IF(XUBND.GT.1.0D0) IEXIT=1
      IF(IEXIT.EQ.1) XUBND=1.0D0
      DUMMY(1)=EF
      CALL QUAD1(DIST,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   20 CONTINUE
      ANS=3.0D0*SUM*((EF0/EF)**(-3.0D0/2.0D0))/2.0D0
C
      A(J)=DLOG10(ANS)
      B(J)=XEXP
```

```
      WRITE(LUOUT,1111) EF,EF0,XEXP,ANS,RATIO
 1111 FORMAT(1X,'EF=',1PD12.5,3X,'EF0=',1PD12.5,3X,'XEXP=',1PD10.2,
     $3X,'ANS=',1PD12.5,3X,'EB/EF=',1PD9.2)
      XEXP=XEXP+TDLT
   30 CONTINUE
      WRITE(LUOUT)
      RATIO=RATIO+RDLT
   40 CONTINUE
C
      END
```

```
C     ================================================================
C     SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
C                       LEGENDRE TYPE
C
C
C     USEAGE: CALL QUAD1(FUNC,XLBND,XUBND,RES.IAR,DUMMY)
C             FUNC   =FUNCTION TO BE INTEGRATED. THIS FUNCTION
C                     MUST BE OF THE FORM FUNCTION FUNC(ARG.DUMMY)
C             DUMMY  = 1-DIM DUMMY ARRAY FOR PASSING DATA
C                      TO FUNC. THIS ARRAY MUST BE DIMENTIONED
C                      IN THE CALLING PROGRAM.
C .           XLBND  = LOWER BOUND OF THE INTEGRAL
C .           XUBND  = UPPER BOUND OF THE INTEGRAL
C .           RES    = RESULT
C             IAR    = NUMBER OF TERMS IN THE INTEGRATION
C                      (MAX=16,MIN=2)
C
C
C       NOTE:
C .          FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
C .               CALLING PROGRAM
C
C
C     REFERENCE:
C .         NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
C .              CHAPMAN HALL, LONDON, 1961
C
C
C     ================================================================
C     ORIGIONAL:C.L. KENNEDY OCT. 1978
C                  C.L. KENNEDY
C       MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
C              TO 16 TERMS  SEPT 1981
C     ================================================================
C
C
      SUBROUTINE QUAD1(FUNC,XLBND.XUBND.RES,IAR,DUMMY)
C
C
      COMMON /QUAD/ Z(8.16),W(8.16)
```

```
      DIMENSION DUMMY(*)

      DATA Z   8*0.0D0,
     $1.5773502691896260,7*0.0D0,
     $0.7745966692414830,7*0.0D0,
     $0.8611363115940530,0.3399810435848560,6*0.0D0,
     $0.9061798459386640,0.5384693101056830,6*0.0D0,
     $0.9324695142031520,0.6612093846626500,0.2386191860831970,5*0.0D0,
     $0.9491079123427590,0.7415311855993940,0.4058451513773970,5*0.0D0,
     $0.9602898564975360,0.7966664774136270,0.5255324099163290,
     $0.1834346424956500,4*0.0D0,
     $0.9681602395076260,0.8360311073266360,0.6133714327805790D0,
     $0.3242534234038090,4*0.0D0,
     $0.9739065285171720,0.8650633666889850,0.6794095682990240,
     $0.4333953941292470,0.1488743389816310,3*0.0D0,
     $0.9782286581460570,0.8870625997680950,0.7301520055740490,
     $0.5199612920681200,0.2695431559523450,3*0.0D0,
     $0.9815606342467190,0.9041172563704750,0.7699026741943050,
     $0.5873179542866170,0.3678314989981800,0.1252334085114690.
     $2*0.0D0,
     $0.9841830547185880,0.9175983992229780,0.8015780907333100,
     $0.6423493394403400,0.4484927510364470,0.2304583159551350.
     $2*0.0D0,
     $0.9862838086968120,0.9284348836635740,0.8272013150697650,
     $0.6872929048116850,0.5152486363581540,0.3191123689278900,
     $0.1080549487073440,0.0D0,
     $0.9879992518020485D0,0.9372733924000706D0,0.8482065834104270,
     $0.7244177313601700,0.5709721726085390,0.3941513470775630,
     $0.2011940939974350,0.0D0,
     $0.9894009349916500,0.9445750230732330,0.8656312023878320,
     $0.7554044083550030,0.6178762444026440,0.4580167776572270,
     $0.2816035507792590,0.0950125098376370/
C
      DATA W / 8*0.0D0,
     $1.0D0,7*0.0D0,
     $0.5555555555555560,0.8888888888888890,6*0.0D0.
     $0.3478548451374540,0.6521451548625460,6*0.0D0.
     $0.2369268850561890,0.4786286704993660,0.5688888888888890,
     $5*0.0D0,0.1713244923791700,0.3607615730481390.
     $0.4679139345726910,5*0.0D0,0.1294849661688700,
     $0.2797053914892770,0.3818300505051190,0.4179591836734690,
     $4*0.0D0,0.1012285632993760,0.2223810344533740,
```

```
     $Ø.31370664587788700,Ø.36268378337836200.
     $4*Ø.ØDØ,Ø.29127473953157400,Ø.180248160694257DØ.
     $Ø.26061259642293500,Ø.31234707724000300,Ø.33023935500126000.
     $3*Ø.ØDØ,Ø.06667134430868800,Ø.14945134915058100,
     $Ø.21908636251598200,Ø.26926671930999600,Ø.29552422471475300,
     $3*Ø.ØDØ,Ø.03556685671161740Ø,Ø.12558036946490500,
     $Ø.18629021092773400,Ø.23319376459199000,
     $Ø.26280454451024700,Ø.27292508677790100,2*Ø.ØDØ,
     $Ø.04717533638651200,Ø.10693932599531800,Ø.16007832854334600,
     $Ø.20316742672306600,Ø.23349253653835500,Ø.24914704581340300.
     $2*Ø.ØDØ,Ø.04048400476531600.Ø.09212149983772800.
     $Ø.13887351021978700,Ø.17814598076194600,Ø.20781604753680900,
     $Ø.22628318026289700,Ø.23255155323087400,Ø.ØDØ,
     $Ø.03511946033175200,Ø.08015808715976000,Ø.12151857068790300,
     $Ø.15720316715819400.Ø.18553839747793800,Ø.20519846372129600,
     $Ø.21526385346315800,Ø.ØDØ,Ø.03075324199611700,
     $Ø.07036604748810800,Ø.10715922046717200,Ø.13957067792615400,
     $Ø.16626920581699400,Ø.18616100001556200,Ø.19843148532711200.
     $Ø.20257824192556100,Ø.02715245941175400,Ø.06225352393864800,
     $Ø.09515851168249300,Ø.12462897125553400,Ø.14959598881657700.
     $Ø.16915651939500300,Ø.18260341504492400,Ø.18945061045506800/
C
C
C
      SUM=Ø.ØDØ
      DO 1Ø I=1,8
      IF(W(I,IAR).EQ.Ø) GOTO 1Ø
      ARG=(Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.ØDØ
      TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
      ARG=(-Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.ØDØ
      TERM2=Ø.ØDØ
      IF(Z(I,IAR).NE.Ø.ØDØ) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
      SUM=SUM+TERM1+TERM2
   1Ø CONTINUE
C
      RES=SUM*(XUBND-XLBND)/2.ØDØ
C
      RETURN
      END
```

10 / 17 / 1981 10 : 33 : 26 DIST.GV

```
      FUNCTION DIST(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   UNOCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EFC=DUMMY(1)
C
      A=DSQRT(ARG)
      B=EFC*(1.0D0-ARG)
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      DIST=A/DENOM
C
C
      RETURN
      END
```

```
C
C
C     ================================================================
C
C     SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
C
C     USAGE  :   CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     WHERE  :   B(X,DUMMY)  =  ARBITRARY FUNCTION
C
C     .          DUMMY       =  A 10 ELEMENT ARRAY USED FOR PASSING
C     .                         PARAMETERS TO THE FUNCTION "B"
C
C     .          X           =  MIN (MAX) VALUE OF X BEGINING SEARCH
C
C     .          XMAX        =  MAX (MIN) VALUE OF X DURING SEARCH
C
C     .          DELX        =  INITIAL STEP SIZE
C     .                         ( +DELX INCREASES X , -DELX DECREASES X )
C
C     .          EPS         =  PERMITTED FRACTIONAL ERROR
C
C     .          IAR         =  ITERATION METHOD
C     .                         ( IAR = 0  BINARY CHOP )
C     .                         ( IAR = 1  METHOD OF SECANTS )
C
C     .          IER         =  ERROR FLAG
C     .                         ( IER = 1 ROOT FOUND )
C     .                         ( IER = 0 ROOT NOT FOUND )
C
C     COMMENT :  THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
C     .          PROGRAM MUST CLASSIFY THE FUNCTION NAME
C     .          TO BE PASSED THROUGH "B" AS EXTERNAL.
C
C     ================================================================
C     ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
C
C     MOD#1    : AERC  C.L. KENNEDY   NOV. 1978
C     .                  IF X REACHES XMAX SET X=0 AND RETURN
C
```

```
C     MOD#2    : AERC  D.P. KENNEDY NOV 1978
C     .                INTRODUCED ERROR FLAG IER
C
C     MOD#3    : AERC  D.P. KENNEDY  NOV. 1978
C     .                EPS=FRACTIONAL CHANGE IN X
C     .                METHOD OF SECANTS INTRODUCED
C
C     MOD#4    : AERC  C.L. KENNEDY DECEMBER 1978
C     .                ALL DUMMY VARIABLES PASSED
C     .                THROUGH ARRAY DUMMY
C
C     ================================================================
C
C
      SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     #      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION P(2),Q(2),DUMMY(1)
C
      IF (DELX.EQ.0.0D0) GOTO 90
      IER=1
      P(1)=0.0D0
      P(2)=0.0D0
      Q(1)=0.0D0
      Q(2)=0.0D0
      Y=B(X,DUMMY)
      P(1)=X
C
C     ----------------------------------------------------------------
C     S T E P    T O    B R A C K E T    R O O T
C     ----------------------------------------------------------------
C
   10 X=X+DELX
      P(2)=X
      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
```

```
      IF(A.LT.0.000) GOTO 15
      Y=Z
      GOTO 10
C
C     ------------------------------------------------------------------
C     B I N A R Y   C H O P   O R   M E T H O D   O F   S E C A N T S ?
C     ------------------------------------------------------------------
C
   15 DEL=DELX
      IF(IAR.EQ.1) GOTO 60
C
C     ------------------------------------------------------------------
C     B I N A R Y    C H O P
C     ------------------------------------------------------------------
C
   20 Y=Z
      P(1)=P(2)
   30 DEL=DEL/2.0D0
      X=X-DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 40
      GOTO 30
C
   40 Y=Z
      P(1)=P(2)
   50 DEL=DEL/2.0D0
      X=X+DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 20
      GOTO 50
C
C     ------------------------------------------------------------------
```

```
C     M E T H O D   O F   S E C A N T S
C     ------------------------------------------------------------------
C
   60 Q(2)=Z
      P(2)=X
      P(1)=X-DEL
      PREP=P(1)
      Q(1)=B(DUMMY,PREP)
   70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
      YY=B(XX,DUMMY)
      P(1)=P(2)
      Q(1)=Q(2)
      P(2)=XX
      Q(2)=YY
      ERROR=DABS((P(1)-P(2))/P(2))
      IF(ERROR.LE.EPS) GOTO 80
      GOTO 70
   80 X=XX
      RETURN
C
C     ------------------------------------------------------------------
C     E R R O R   R E T U R N   X = 0   I E R = 0
C     ------------------------------------------------------------------
C
   90 X=0.0D0
      IER=0
      RETURN
      END
```

```
      COMPILER DOUBLE PRECISION
C
C     ================================================================
C
C     SUBROUTINE XFERMI IS USED TO CALCULATE  THE FERMI LEVEL
C                     IN A METAL AT A SPECIFIED TEMP
C
C     USEAGE: REQUIRES THE FOLLOWING
C             FUNCTION EFERMI
C             SUBROUTINE ROOT
C             FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.
C
C     ================================================================
C
      SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUOUT)
C
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL EFERMI
C
C
C
C     -----CALCULATE FERMI LEVEL AT ZERO K-----
C
      EF0=3.0D0*ELECT*1.0D-21/(EMASS**(3.0D0/2.0D0)*1.2368D1)
      EF0=EF0**(2.0D0/3.0D0)
      EF0=EF0/(8.617D-5*T)
C
C     -----CALCULATE FERMI LEVEL-----
C
      DUMMY(1)=EF0
      EF=EF0*0.75D0
      EFMAX=1.0D2*EF0
      DELTE=EF0*5.0D-1
      EPS=1.0D-4
C
```

```
      CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1.,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND'
      IF(IER.NE.1) STOP
      END
```

```
C
C     ================================================================
C
C     FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
C                      METALLIC CONDUCTOR
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      FUNCTION EFERMI(EF,DUMMY)
      DIMENSION DUMMY(10)
      EXTERNAL XINT
C
C     -----INTEGRATE FROM 0 TO INF-----
C
      EF0=DUMMY(1)
      DUMMY(2)=EF
      SUM=0.0D0
      XX=EF-1.2D1
      IF(XX.GT.0.0D0) SUM=2.0D0*(XX**(3.0D0/2.0D0))/3.0D0
      XUBND=0.0D0
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      XLBND=XUBND
      XUBND=XUBND+1.0D1
      XX=XUBND-EF
      IF(XX.GT.1.0D2) GOTO 30
      CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   30 CONTINUE
      EFERMI=1.0D0-3.0D0*EF0**(-3.0D0/2.0D0)*SUM/2.0D0
C
C
```

```
      RETURN
      END
```

```
      FUNCTION XINT(ARG,DUMMY)
C
C     ================================================================
C     FUNCTION XINT:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   OCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
C
      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      XINT=A/DENOM
C
C
      RETURN
      END
```

APPENDIX I-D

Program for Calculating Unoccupied Energy States Between the Conduction Band Edge E_c and an Energy E_b Where $(E_c < E_b < E_f)$

```
C
C     ================================================================
C
C     MAIN PROGRAM FOR CALCULATING THE DENSITY OF UNOCCUPIED
C     ENERGY STATES THAT RESIDE BETWEEN THE FERMY LEVEL AND
C     AN ARBITRARY ENERGY EB WHERE EC<EB<EF
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1,FUNCTION DIST, SUBROUTINE ROOT
C              SUBROUTINE XFERMI,FUNCTION FERMI,AND FUNCTION XINT
C
C              TEXP=EXPONENT FOR TEMP STEPPING
C              TDLT=TEMP STEP SIZE
C              JMAX=NUMBER OF TEMP STEPS
C              RATIO=EB/EF RATIO
C              RDLT=STEP SIZE FOR RATIO
C              IMAX=MAX. NUMBER OF STEPS FOR RATIO
C              ELECT=FREE ELECTRON DENSITY
C              EMASS=ELECTRON MASS RATIO (M*/M)
C
C
C              LUOUT=CHANNEL FOR OUTPUT
C
C
C     ================================================================
C
C     ORIGINAL: D.F. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL DIST
C
C     -----INITIALIZE MISC CONSTANTS-----
C

      TEXP=-2.5
      TDLT=1.0D-1
      JMAX=13
      ELECT=1.0D23
      EMASS=1.0D0
```

```
      RATIO=0.'12
      RDLT=1.0D-'
      IMAX=13
      LUOUT=10
C
C     -----TOP OF EB/EF STEPPING LOOP-----
C
      DO 40 I=1,IMAX
C
C     -----TOP OF TEMP STEPPING LOOP-----
C
      XEXP=TEXP
      DO 30 J=1,JMAX
      T=1.0D1**(-XEXP)
C
C     -----CALCULATE FERMI LEVEL-----
C
      CALL XFERMI(ELECT,EF0,T,EMASS,EF,LUOUT)
C
C     -----INTEGRATE FROM EB TO EF-----
C
      IEXIT=0
      SUM=0.0D0
      XUBND=1.0D0-1.2D1/EF
      IF(XUBND.LT.RATIO) XUBND=RATIO
   10 CONTINUE
      IF(IEXIT.EQ.1) GOTO 20
      XLBND=XUBND
      XUBND=XUBND+1.0D-2
      IF(EF.GT.5.0D2) XUBND=XUBND+1.0D-3
      IF(XUBND.GT.1.0D0) IEXIT=1
      IF(IEXIT.EQ.1) XUBND=1.0D0
      DUMMY(1)=EF
      CALL QUAD1(DIST,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   20 CONTINUE
      ANS=3.0D0*SUM*((EF0/EF)**(-3.0D0/2.0D0))/2.0D0
C
      A(J)=DLOG10(ANS)
      B(J)=XEXP
```

```
      WRITE(LUOUT,1111) EF,EF0,XEXP,ANS,RATIO
 1111 FORMAT(1X,'EF=',1PD12.5,3X,'EF0=',1PD12.5,3X,'XEXP= ',1PD10.2,
     &3X, ANS=',1PD12.5,3X,'ES/EF=',1PD9.2)
      XEXP=XEXP+TDLT
   30 CONTINUE
      WRITE(LUOUT)
C
      RATIO=RATIO+RDLT
   40 CONTINUE
      END
```

```
C     ================================================================
C     SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
C                       LEGENDRE TYPE
C
C
C     USEAGE: CALL QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C             FUNC   =FUNCTION TO BE INTEGRATED. THIS FUNCTION
C                     MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
C             DUMMY  = 1-DIM DUMMY ARRAY FOR PASSING DATA
C                      TO FUNC. THIS ARRAY MUST BE DIMENTIONED
C                      IN THE CALLING PROGRAM.
C .           XLBND  = LOWER BOUND OF THE INTEGRAL
C .           XUBND  = UPPER BOUND OF THE INTEGRAL
C .           RES    = RESULT
C             IAR    = NUMBER OF TERMS IN THE INTEGRATION
C                      (MAX=16,MIN=2)
C
C
C       NOTE:
C .          FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
C .               CALLING PROGRAM
C
C
C     REFERENCE:
C .          NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
C .               CHAPMAN HALL, LONDON, 1961
C
C
C     ================================================================
C     ORIGIONAL:C.L. KENNEDY OCT. 1978
C                  C.L. KENNEDY
C       MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
C             TO 16 TERMS  SEPT 1981
C     ================================================================
C
C
      SUBROUTINE QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C
C
      COMMON /QUAD/ Z(8,16),W(8,16)
```

```
      DIMENSION X(**).W(**)
C
      DATA X / 8*0.D0,
     $.57735026918962D0,7*0.0D0,
     $0.77459666924148D0,7*0.0D0,
     $0.86113631159405D0,0.33998104358485D0,6*0.0D0,
     $0.90617984593866D0,0.53846931010568D0,6*0.0D0,
     $0.93246951420315D0,0.66120938646626D0,0.23861918608319D0,5*0.0D0,
     $0.94910791234276D0,0.74153118559939D0,0.40584515137739D0,5*0.0D0,
     $0.96028985649753D0,0.79666477413627D0,0.52553240991632D0,
     $0.18343464249565D0,4*0.0D0,
     $0.96816023950762D0,0.83603110732663D0,0.61337143270059D0,
     $0.32425342340380D0,4*0.0D0,
     $0.97390652851717D0,0.86506336668898D0,0.67940956829902D0,
     $0.43339539412924D0,0.14887433898163D0,3*0.0D0,
     $0.97822865814605D0,0.88706259976809D0,0.73015200557404D0,
     $0.51909612920681D0,0.26954315595234D0,3*0.0D0,
     $0.98156063424671D0,0.90411725637047D0,0.76990267419430D0,
     $0.58731795428661D0,0.36783149899818D0,0.12523340851146D0,
     $2*0.0D0,
     $0.98418305471858D0,0.91759839922297D0,0.80157809073310D0,
     $0.64234933944034D0,0.44849275103644D0,0.23045831595513D0,
     $2*0.0D0,
     $0.98628380869681D0,0.92843488366357D0,0.82720131506976D0,
     $0.68729290481168D0,0.51524863635815D0,0.31911236892789D0,
     $0.10805494870734D0,0.0D0,
     $0.98799251802485D0,0.93727339240070D0,0.84820658341042D0,
     $0.72441773136817D0,0.57097217260853D0,0.39415134707756D0,
     $0.20119409399743D0,0.0D0,
     $0.98940093499165D0,0.94457502307323D0,0.86563120238732D0,
     $0.75540440835503D0,0.61787624440264D0,0.45801677765722D0,
     $0.28160355077925D0,0.09501250983763D0/
C
      DATA W / 8*0.0D0,
     $1.0D0,7*0.0D0,
     $0.55555555555556D0,0.88888888888889D0,6*0.0D0,
     $0.34785484513745D0,0.65214515486255D0,6*0.0D0,
     $0.23692688505619D0,0.47862867049936D0,0.56888888888889D0,
     $5*0.0D0,0.17132449237917D0,0.36076157304814D0,
     $0.46791393457269D0,5*0.0D0,0.12948496616887D0,
     $0.27970539148927D0,0.38183005050511D0,0.41795918367347D0,
     $4*0.0D0,0.10122856329038D0,0.22238103445337D0,
```

```
     $0.313706645877887D0,0.362683783378362D0,
     $4*0.0D0,0.081274388361574D0,0.180648160694857D0,
     $0.260610696402935D0,0.312347077040023D0,0.330239355001260D0,
     $3*0.0D0,0.366571344308688D0,0.149451349150581D0,
     $0.219086362515982D0,0.269266719309996D0,0.295524224714753D0,
     $3*0.0D0,0.055668567116174D0,0.125580369464905D0,
     $0.186290210927734D0,0.233193764591990D0,
     $0.262804544510247D0,0.272925086777901D0,2*0.0D0,
     $0.047175336386512D0,0.106939325995318D0,0.160078328543346D0,
     $0.203167426723066D0,0.233492536538355D0,0.249147045813403D0,
     $2*0.0D0,0.040484004765316D0,0.092121499837728D0,
     $0.138873510219787D0,0.178145980761946D0,0.207816047536889D0,
     $0.226283180262897D0,0.232551553230874D0,0.0D0,
     $0.035119460331752D0,0.080158087159760D0,0.121518570687903D0,
     $0.157203167158194D0,0.185538397477938D0,0.205198463721296D0,
     $0.215263853463158D0,0.0D0,0.030753241996117D0,
     $0.070366047488108D0,0.107159220467172D0,0.139570677926154D0,
     $0.166269205816994D0,0.186161000015562D0,0.198431485327112D0,
     $0.202578241925561D0,0.027152459411754D0,0.062253523938648D0,
     $0.095158511682493D0,0.124628971255534D0,0.149595988816577D0,
     $0.169156519395003D0,0.182603415044924D0,0.189450610455068D0/
C
C
C
      SUM=0.0D0
      DO 10 I=1,8
      IF(W(I,IAR).EQ.0) GOTO 10
      ARG=(Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
      ARG=(-Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM2=0.0D0
      IF(Z(I,IAR).NE.0.0D0) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
      SUM=SUM+TERM1+TERM2
   10 CONTINUE
C
      RES=SUM*(XUBND-XLBND)/2.0D0
C
      RETURN
      END
```

```
      FUNCTION DIST(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   UNOCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EFC=DUMMY(1)
C
      A=DSQRT(ARG)
      B=EFC*(1.0D0-ARG)
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      DIST=A/DENOM
C
C
      RETURN
      END
```

```
C
C     ================================================================
C
C     SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
C
C     USAGE  :   CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     WHERE  :   B(X,DUMMY)  =  ARBITRARY FUNCTION
C
C     .          DUMMY       =  A 10 ELEMENT ARRAY USED FOR PASSING
C     .                         PARAMETERS TO THE FUNCTION "B"
C
C     .          X           =  MIN (MAX) VALUE OF X BEGINING SEARCH
C
C     .          XMAX        =  MAX (MIN) VALUE OF X DURING SEARCH
C
C     .          DELX        =  INITIAL STEP SIZE
C     .                         ( +DELX INCREASES X , -DELX DECREASES X )
C
C     .          EPS         =  PERMITTED FRACTIONAL ERROR
C
C     .          IAR         =  ITERATION METHOD
C     .                         ( IAR = 0  BINARY CHOP )
C     .                         ( IAR = 1  METHOD OF SECANTS )
C
C     .          IER         =  ERROR FLAG
C     .                         ( IER = 1 ROOT FOUND )
C     .                         ( IER = 0 ROOT NOT FOUND )
C
C     COMMENT :  THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
C     .          PROGRAM MUST CLASSIFY THE FUNCTION NAME
C     .          TO BE PASSED THROUGH "B" AS EXTERNAL.
C
C     ================================================================
C     ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
C
C     MOD#1    : AERC  C.L. KENNEDY   NOV. 1978
C     .                  IF X REACHES XMAX SET X=0 AND RETURN
C
```

```
C     MOD#2    : AERE  D.P. KENNEDY NOV 1978
C     .                    INTRODUCED ERROR FLAG IER
C
C     MOD#3    : AERE  D.P. KENNEDY  NOV. 1978
C     .                    EPS=FRACTIONAL CHANGE IN X
C     .                    METHOD OF SECANTS INTRODUCED
C
C     MOD#4    : AERE  D.P. KENNEDY DECEMBER 1978
C     .                    ALL DUMMY VARIABLES PASSED
C     .                    THROUGH ARRAY DUMMY
C
C     ================================================================
C
      SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     #      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION P(2),Q(2),DUMMY(1)
C
      IF (DELX.EQ.0.0D0) GOTO 90
      IER=1
      P(1)=0.0D0
      P(2)=0.0D0
      Q(1)=0.0D0
      Q(2)=0.0D0
      Y=B(X,DUMMY)
      P(1)=X
C     ----------------------------------------------------------------
C     S T E P   T O   B R A C K E T   R O O T
C     ----------------------------------------------------------------
C
   10 X=X+DELX
      P(2)=X
      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
```

```
      IF(A.LT.0.0D0) GOTO 15
      Y=Z
      GOTO 10
C
C     ------------------------------------------------------------------
C     B I N A R Y   C H O P   O R   M E T H O D   O F   S E C A N T S ?
C     ------------------------------------------------------------------
C
   15 DEL=DELX
      IF(IAR.EQ.1) GOTO 60
C
C     ------------------------------------------------------------------
C     B I N A R Y    C H O P
C     ------------------------------------------------------------------
C
   20 Y=Z
      P(1)=P(2)
   30 DEL=DEL/2.0D0
      X=X-DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 40
      GOTO 30
C
   40 Y=Z
      P(1)=P(2)
   50 DEL=DEL/2.0D0
      X=X+DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 20
      GOTO 50
C
C     ------------------------------------------------------------------
```

```
C     M E T H O D   O F   S E C A N T S
C     ------------------------------------------------------------
C
C
   6Ø Q(2)=Z
      P(2)=X
      P(1)=X-DEL
      PREP=P(1)
      Q(1)=B(DUMMY,PREP)
   7Ø XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
      YY=B(XX,DUMMY)
      P(1)=P(2)
      Q(1)=Q(2)
      P(2)=XX
      Q(2)=YY
      ERROR=DABS((P(1)-P(2))/P(2))
      IF(ERROR.LE.EPS) GOTO 8Ø
      GOTO 7Ø
   8Ø X=XX
      RETURN
C
C     ------------------------------------------------------------
C     E R R O R   R E T U R N   X = Ø   I E R = Ø
C     ------------------------------------------------------------
C
   9Ø X=Ø.ØDØ
      IER=Ø
      RETURN
      END
```

```
C
C     ================================================================
C
C     FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
C                      METALLIC CONDUCTOR
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.F. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      FUNCTION EFERMI(EF,DUMMY)
      DIMENSION DUMMY(10)
      EXTERNAL XINT
C
C     -----INTEGRATE FROM 0 TO INF-----
C
      EF0=DUMMY(1)
      DUMMY(2)=EF
      SUM=0.0D0
      XX=EF-1.2D1
      IF(XX.GT.0.0D0) SUM=2.0D0*(XX**(3.0D0/2.0D0))/3.0D0
      XUBND=0.0D0
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      XLBND=XUBND
      XUBND=XUBND+1.0D1
      XX=XUBND-EF
      IF(XX.GT.1.0D2) GOTO 30
      CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   30 CONTINUE
      EFERMI=1.0D0-3.0D0*EF0**(-3.0D0/2.0D0)+SUM/2.0D0
C
C
```

```
RETURN
END
```

```
      FUNCTION XINT(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION XINT:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   OCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
C
      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      XINT=A/DENOM
C
C
      RETURN
      END
```

```
      COMPILER DOUBLE PRECISION
      ================================================================
C
C     SUBROUTINE XFERMI IS USED TO CALCULATE  THE FERMI LEVEL
C                     IN A METAL AT A SPECIFIED TEMP
C
C     USEAGE: REQUIRES THE FOLLOWING
C             FUNCTION EFERMI
C             SUBROUTINE ROOT
C             FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.
C
C     ================================================================
C
      SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUOUT)
C
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL EFERMI
C
C
C
C     -----CALCULATE FERMI LEVEL AT ZERO K------
C
      EF0=3.0D0*ELECT*1.0D-21/(EMASS**(3.0D0/2.0D0)*1.2368D1)
      EF0=EF0**(2.0D0/3.0D0)
      EF0=EF0/(8.617D-5*T)
C
C     -----CALCULATE FERMI LEVEL-----
C
      DUMMY(1)=EF0
      EF=EF0*0.75D0
      EFMAX=1.0D2*EF0
      DELTE=EF0*5.0D-1
      EPS=1.0D-4
C
```

```
      CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT) 'ROOT NOT FOUND'
      IF(IER.NE.1) STOP
      END
```

APPENDIX I-E

Program for Calculating the Transition Energy W_t in a Metal-Semiconductor Contact.

```
C     ================================================================
C
C     MAIN PROGRAM FOR CALCULATING THE TRANSITION ENERGY IN A
C     P-TYPE SHOTTKY BARRIER
C
C     USEAGE: REQUIRES THE SUBROUTINES
C             SUBROUTINE ROOT
C             FUNCTION DIST
C             FUNCTION ZERO
C             SUBROUTINE XFERMI
C             FUNCTION EFERMI
C             SUBROUTINE QUAD1
C             FUNCTION XINT
C
C
C              TEXP=EXPONENT FOR TEMP STEPPING
C              TDLT=TEMP STEP SIZE
C              JMAX=NUMBER OF TEMP STEPS
C              WC=(EF-EC) START OF STEPPING
C              WDLT=STEP SIZE FOR WC
C              IMAX=MAX. NUMBER OF STEPS FOR WC
C              EMASS=ELECTRON MASS RATIO (M*/M) FOR METAL
C              FELECT=FREE ELECTRON DENSITY IN METAL
C              VELECT=VALENCE ELECTRON DENSITY IN SEMI.
C
C
C              LUOUT=CHANNEL FOR OUTPUT
C
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL ZERO,DIST
C
C     -----INITIALIZE MISC CONSTANTS-----
```

```
      XMASS=9.1085D-34
      BOLTZ=8.61667D-5
      FELECT=1.0D22
      VELECT=1.0D23
      TEXP=-2.4
      TDLT=1.0D-1
      JMAX=12
      EMASS=1.0D0
      WC=1.0D0
      WDLT=1.0D-1
      IMAX=10
      LUOUT=10
C
C     -----TOP OF WC STEPPING LOOP-----
C
      DO 40 I=1,IMAX
      WRITE(10) 'WC=',WC
C
C     -----TOP OF TEMP STEPPING LOOP-----
C
      XEXP=TEXP
      DO 30 J=1,JMAX
      T=1.0D1**(-XEXP)
C
C     -----CALCULATE FERMI LEVEL FOR METAL----
C
      CALL XFERMI(FELECT,EF0,T,EMASS,EF,LUOUT)
      RATIO=1.0D0-WC/(EF*BOLTZ*T)
C
C     ----CALC SILICON FERMI LEVEL AT ZERO DEG K-----
C
      SEF0=3.0D0*VELECT*1.0D-21/(SEMASS**(3.0D0/2.0D0)*1.2368D1)
      SEF0=SEF0**(2.0D0/3.0D0)
      SEF0=SEF0/(8.67D-5*T)
C
C     -----CALC DENSITY OF UNOCCUPIED STATES IN VALENCE BAND-----
C
      IEXIT=0
      SUM=0.0D0
      XX=SEF0+EF*(1.0D0-RATIO)
```

```
      XUBND=1.ØD0-1.ØD2/XX
      IF(XUBND.LT.Ø.ØD0) XUBND=Ø.ØD0
      EC=SEFØ
   25 CONTINUE
      IF(IEXIT.EQ.1) GOTO 27
      XLBND=XUBND
      XUBND=XUBND+1.ØD1/XX
      IF(XUBND.GT.EC/XX) IEXIT=1
      IF(IEXIT.EQ.1) XUBND=EC/XX
      DUMMY(1)=XX
      CALL QUAD1(DIST,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      IF(SUM.LT.1.ØD-6Ø) SUM=1.ØD-6Ø
      GOTO 25
C
   27 CONTINUE
      YY=3.ØD0/2.ØD0
      XNV=DLOG(3.ØD0/2.ØD0)+DLOG(VELECT)-YY*DLOG(SEFØ/XX)
      XNV=XNV+DLOG(SUM)
      IF(XNV.LT.-1.6D2) XNV=-1.6D2
      XNV=DEXP(XNV)
      P=SEFØ*BOLTZ*T
C     WRITE(1Ø,1122) P,XNV
 1122 FORMAT(1X,'SEFØ=',1PD11.4,3X,'XNV=',1PD11.4)
C
C     -----CALC.ET-----
C
      DUMMY(1)=FELECT
      DUMMY(2)=RATIO
      DUMMY(3)=EF
      DUMMY(4)=XMASS
      DUMMY(5)=EFØ
      DUMMY(6)=XNV
      DUMMY(7)=T
C
      ARG=EF*RATIO
      IF(ARG.LT.Ø.ØD0) ARG=Ø.ØD0
      XX=ZERO(ARG,DUMMY)
      IF(XX.GE.Ø.ØD0) ET=ARG
      IF(XX.GE.Ø.ØD0) GOTO 5
C
      ET=Ø.ØD0
```

```
      ETMAX=1.ØD2*EF
      DLTE=EF/10.ØDØ
      EPS=1.ØD-4
C
      CALL ROOT(ZERO,ET,ETMAX,DLTE,EPS,Ø,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT)'ROOT FOR ET NOT FOUND'
      IF(IER.NE.1) STOP
C
    5 CONTINUE
C
      EB=RATIO*EF
      WT=(ET-EF*RATIO)*BOLTZ*T
      A(J)=WT
      B(J)=XEXP
      WRITE(LUOUT,1111) EF,EFØ,XEXP,ET,EB,WT
 1111 FORMAT(1X,'EF=',1PD12.5,3X,'EFØ=',1PD12.5,3X,'TEMP=',1PD1Ø.2,
     &3X,'ET=',1PD12.5,3X,'EB=',1PD12.5,3X,'WT=',1PD12.5)
      XEXP=XEXP*DLT
   30 CONTINUE
      WRITE(LUOUT)
C
      WC=WC-WDLT
   40 CONTINUE
      END
```

```
C
C
C     ================================================================
C
C     SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
C
C     USAGE  :   CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     WHERE  :   B(X,DUMMY)  =  ARBITRARY FUNCTION
C
C     .          DUMMY       =  A 10 ELEMENT ARRAY USED FOR PASSING
C     .                         PARAMETERS TO THE FUNCTION "B"
C
C     .          X           =  MIN (MAX) VALUE OF X BEGINING SEARCH
C
C     .          XMAX        =  MAX (MIN) VALUE OF X DURING SEARCH
C
C     .          DELX        =  INITIAL STEP SIZE
C     .                         ( +DELX INCREASES X , -DELX DECREASES X )
C
C     .          EPS         =  PERMITTED FRACTIONAL ERROR
C
C     .          IAR         =  ITERATION METHOD
C     .                         ( IAR = 0  BINARY CHOP )
C     .                         ( IAR = 1  METHOD OF SECANTS )
C
C     .          IER         =  ERROR FLAG
C     .                         ( IER = 1 ROOT FOUND )
C     .                         ( IER = 0 ROOT NOT FOUND )
C
C     COMMENT :  THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
C     .          PROGRAM MUST CLASSIFY THE FUNCTION NAME
C     .          TO BE PASSED THROUGH "B" AS EXTERNAL.
C
C     ================================================================
C     ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
C     MOD#1    : AERC  C.L. KENNEDY   NOV. 1978
C     .                  IF X REACHES XMAX SET X=0 AND RETURN
C
```

```
C     MOD#2    : AERE  D.P. KENNEDY NOV 1978
C     .                    INTRODUCED ERROR FLAG IER
C
C     MOD#3    : AERE  D.P. KENNEDY  NOV. 1978
C     .                    EPS=FRACTIONAL CHANGE IN X
C     .                    METHOD OF SECANTS INTRODUCED
C
C     MOD#4    : AERE  C.L. KENNEDY DECEMBER 1978
C     .                    ALL DUMMY VARIABLES PASSED
C     .                    THROUGH ARRAY DUMMY
C
C     ================================================================
C
C
      SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     #      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION P(2),Q(2),DUMMY(1)
C
      IF (DELX.EQ.0.0D0) GOTO 90
      IER=1
      P(1)=0.0D0
      P(2)=0.0D0
      Q(1)=0.0D0
      Q(2)=0.0D0
      Y=B(X,DUMMY)
      P(1)=X
C
C     ----------------------------------------------------------------
C     S T E P   T O   B R A C K E T   R O O T
C     ----------------------------------------------------------------
C
   10 X=X+DELX
      P(2)=X
      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
```

```
      IF(A.LT.0.0D0) GOTO 15
      Y=Z
      GOTO 10
C
C     ------------------------------------------------------------------
C     B I N A R Y   C H O P   O R   M E T H O D   O F   S E C A N T S ?
C     ------------------------------------------------------------------
C
   15 DEL=DELX
      IF(IAR.EQ.1) GOTO 60
C
C     ------------------------------------------------------------------
C     B I N A R Y    C H O P
C     ------------------------------------------------------------------
C
   20 Y=Z
      P(1)=P(2)
   30 DEL=DEL/2.0D0
      X=X-DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 40
      GOTO 30
C
   40 Y=Z
      P(1)=P(2)
   50 DEL=DEL/2.0D0
      X=X+DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 20
      GOTO 50
C
C     ------------------------------------------------------------------
```

```
C     M E T H O D   O F   S E C A N T S
C     ---------------------------------------------------------------
C
   60 Q(2)=Z
      P(2)=X
      P(1)=X-DEL
      PREP=P(1)
      Q(1)=B(DUMMY,PREP)
   70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
      YY=B(XX,DUMMY)
      P(1)=P(2)
      Q(1)=Q(2)
      P(2)=XX
      Q(2)=YY
      ERROR=DABS((P(1)-P(2))/P(2))
      IF(ERROR.LE.EPS) GOTO 80
      GOTO 70
   80 X=XX
      RETURN
C
C     ---------------------------------------------------------------
C     E R R O R   R E T U R N   X = 0   I E R = 0
C     ---------------------------------------------------------------
C
   90 X=0.0D0
      IER=0
      RETURN
      END
```

```
      FUNCTION DIST ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   UNOCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EFC=DUMMY(1)
C
      A=DSQRT(ARG)
      B=EFC*(1.0D0-ARG)
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      DIST=A/DENOM
C
C
      RETURN
      END
```

```
C
C     ================================================
C     FUNCTION ZERO: CALCULATES WITHIN AN ENERGY RANGE E AND
C                    (E+DE) THE DIFFERENCE BETWEEN UNOCCUPIED
C                    STATES IN THE METAL AND ELECTRONS WITH
C                    A MAXWELLIAN DISTRIBUTION THAT ARE
C                    AVAILABLE TO OCCUPY THESE STATES
C
C     ================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE, FLA.
C
C     ================================================
C
      FUNCTION ZERO(ARG,DUMMY)
      DIMENSION DUMMY(10)
      FELECT=DUMMY(1)
      EF=DUMMY(3)
      XNV=DUMMY(6)
      T=DUMMY(7)
      BOLTZ=8.61666D0
      PI=3.14159265
C
C
      XX=ARG
      IF(DABS(XX).LE.1.0D-70) XX=1.0D-70
      TERM1=DLOG(3.0D0)+DLOG(FELECT)-3.0D0*DLOG(EF0)/2.0D0+DLOG(XX)
      XX=EF-ARG
      IF(XX.GT.1.5D2) TERM1=TERM1-XX
      IF(XX.GT.1.5D2) GOTO 10
      IF(XX.LT.-1.5D2) GOTO 10
      TERM1=TERM1-DLOG(1.0D0+DEXP(XX))
   10 CONTINUE
C
C
      TERM2=-DLOG(DSQRT(1.0D0/(2.0D0*PI*BOLTZ*T)))+DLOG(XNV)
      XX=ARG-RATIO*EF
      TERM2=TERM2-XX

      ZERO=TERM1-TERM2
```

```
      RETURN
      END
```

```
      COMPILER DOUBLE PRECISION
C
C     ================================================================
C
C     SUBROUTINE XFERMI IS USED TO CALCULATE  THE FERMI LEVEL
C                     IN A METAL AT A SPECIFIED TEMP
C
C     USEAGE: REQUIRES THE FOLLOWING
C             FUNCTION EFERMI
C             SUBROUTINE ROOT
C             FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC.. GAINESVILLE FLA.
C
C     ================================================================
C
      SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUOUT)
C
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL EFERMI
C
C
C
C     -----CALCULATE FERMI LEVEL AT ZERO K-----
C
      EF0=3.0D0*ELECT*1.0D-21/(EMASS**(3.0D0/2.0D0)*1.2368D1)
      EF0=EF0**(2.0D0/3.0D0)
      EF0=EF0/(8.617D-5*T)
C
C     -----CALCULATE FERMI LEVEL-----
C
      DUMMY(1)=EF0
      EF=EF0*0.75D0
      EFMAX=1.0D2*EF0
      DELTE=EF0*5.0D-1
      EPS=1.0D-4
C
```

```
      CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND'
      IF(IER.NE.1) STOP
      END
```

```
C
C     ================================================================
C
C     FUNCTION EFERMI: IS USED TO CALC. THE FERM. LEVEL IN A
C                      METALLIC CONDUCTOR
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      FUNCTION EFERMI(EF,DUMMY)
      DIMENSION DUMMY(10)
      EXTERNAL XINT
C
C     -----INTEGRATE FROM 0 TO INF-----
C
      EF0=DUMMY(1)
      DUMMY(2)=EF
      SUM=0.0D0
      XX=EF-1.2D1
      IF(XX.GT.0.0D0) SUM=2.0D0*(XX**(3.0D0/2.0D0))/3.0D0
      XUBND=0.0D0
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      XLBND=XUBND
      XUBND=XUBND+1.0D1
      XX=XUBND-EF
      IF(XX.GT.1.0D2) GOTO 30
      CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   30 CONTINUE
      EFERMI=1.0D0-3.0D0*EF0**(-3.0D0/2.0D0)*SUM/2.0D0
C
C
```

```
      RETURN
      END
```

```
C     ================================================================
C     SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
C                       LEGENDRE TYPE
C
C
C     USEAGE: CALL QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C             FUNC   =FUNCTION TO BE INTEGRATED. THIS FUNCTION
C                     MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
C             DUMMY  = 1-DIM DUMMY ARRAY FOR PASSING DATA
C                      TO FUNC. THIS ARRAY MUST BE DIMENTIONED
C                      IN THE CALLING PROGRAM.
C .           XLBND  = LOWER BOUND OF THE INTEGRAL
C .           XUBND  = UPPER BOUND OF THE INTEGRAL
C .           RES    = RESULT
C             IAR    = NUMBER OF TERMS IN THE INTEGRATION
C                      (MAX=16,MIN=2)
C
C
C       NOTE:
C .          FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
C .               CALLING PROGRAM
C
C
C     REFERENCE:
C .          NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
C .               CHAPMAN HALL, LONDON, 1961
C
C
C     ================================================================
C     ORIGIONAL:C.L. KENNEDY OCT. 1978
C                   C.L. KENNEDY
C       MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
C            TO 16 TERMS  SEPT 1981
C     ================================================================
C
C
      SUBROUTINE QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C
C
      COMMON /QUAD/ Z(8,16),W(8,16)
```

```
      DIMENSION DUMMY(1)
C
      DATA Z / 8*0.0D0,
     $3.5[illegible]2691896260,7*0.0D0,
     $0.7745966692414830,7*0.0D0,
     $0.8611363115940530,0.3399810435848560,6*0.0D0,
     $0.9061798459386640,0.5384693101056830,6*0.0D0,
     $0.9324695142031520,0.6612093864662650,0.2386[illegible]860831970,5*0.0D0,
     $0.9491[illegible]9123427590,0.7415311855993940,0.4058451513773970,5*0.0D0,
     $0.9602898564975360,0.7966664774136270,0.5255324099163290,
     $0.1834346424956500,4*0.0D0,
     $0.9681602395076260,0.8360311[illegible]326360,0.6133714327005900,
     $0.3242534234038090,4*0.0D0,
     $0.9739065285171720,0.8650633666889850,0.6794095682990240,
     $0.4333953941292470,0.1488743389816310,3*0.0D0,
     $0.9782286581460570,0.8870625997680950,0.7301520055740490,
     $0.5190961292068120,0.2695431559523450,3*0.0D0,
     $0.9815606342467190,0.9041172563704750,0.7699026741943050,
     $0.5873179542866170,0.3678314989981800,0.1252334085111469D0,
     $2*0.0D0,
     $0.9841830547185880,0.9175983992229780,0.8015780907333100,
     $0.6423493394403400,0.4484927510364470,0.2304583159551350,
     $2*0.0D0,
     $0.9862838086968120,0.9284348836635740,0.8272013150697650,
     $0.6872929048116850,0.5152486363581540,0.3191123689278900,
     $0.1080549437073440,0.0D0,
     $0.9879925180204850,0.9372733924007060,0.8482065831104270,
     $0.7244177313601700,0.5709721726085390,0.3941513470775630,
     $0.2011940939974350,0.0D0,
     $0.9894009349916500,0.9445750230732330,0.8656312023878320,
     $0.7554044083550030,0.6178762444026440,0.4580167776572270,
     $0.2816035507792590,0.0950125098376370/
C
      DATA W / 8*0.0D0,
     $1.0D0,7*0.0D0,
     $0.5555555555555560,0.8888888888888890,6*0.0D0,
     $0.3478548451374540,0 6521451548625460.6*0.0D0,
     $0.2369268850561890,0.4786286704993660.0.5688888888888890.
     $5*0.0D0,0.1713244923791700,0.3607615730481390,
     $0.4679139345726910.5*0.0D0,0.1294849661688700.
     $0.2797053914892770,0.3818300505051190.0.4179591836734690.
     $4*0.0D0,0.1012285632903760,0.2223810344533740.
```

```
     $0.3137066458778870,0.3626837833783620,
     $4*0.0D0,0.0812743883615740,0.1806481686948570,
     $0.2606106964029350,0.3123470770400030,0.3302393559001260D0,
     $3*0.0D0,0.0666713443086880,0.1494513491585810,
     $0.2190863625159820,0.2692667193099960,0.2955242247147530,
     $3*0.0D0,0.0556685671617400,0.1255803694649950,
     $0.1862902109277340,0.2331937645919900,
     $0.2628045445102470,0.2729250867779010,2*0.0D0,
     $0.0471753363865120,0.1069393259953180,0.1600783285433460,
     $0.2031674267230660,0.2334925365383550,0.2491470458134030,
     $2*0.0D0,0.0404840047653160,0.0921214998377280,
     $0.1388735102197870,0.1781459807619460,0.2078160475368890,
     $0.2262831802628970,0.2325515532308740,0.0D0,
     $0.0351194603317520,0.0801588715976000,0.1215185706879030,
     $0.1572031671581940,0.1855383974779380,0.2051984637212960,
     $0.2152638534631580,0.0D0,0.0307532419961170,
     $0.0703660474881080,0.1071592204671720,0.1395706779261540,
     $0.1662692058169940,0.1861610000155620,0.1984314853271120,
     $0.2025782419255610,0.0271524594117540,0.0622535239386480,
     $0.0951585116824930,0.1246289712555340,0.1495959888165770,
     $0.1691565193950030,0.1826034150449240,0.1894506104550680/
C
C
C
      SUM=0.0D0
      DO 10 I=1,8
      IF(W(I,IAR).EQ.0) GOTO 10
      ARG=(Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
      ARG=(-Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM2=0.0D0
      IF(Z(I,IAR).NE.0.0D0) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
      SUM=SUM+TERM1+TERM2
   10 CONTINUE
C
      RES=SUM*(XUBND-XLBND)/2.0D0
C
      RETURN
      END
```

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```
      FUNCTION XINT(ARG,DUMMY)
C     ================================================================
C
C     FUNCTION XINT:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   OCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
C
      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      XINT=A/DENOM
C
C
      RETURN
      END
```

APPENDIX I-F

Program for Calculating the Saturation Current Components J_1 and J_2, and the Saturation Current Using Conventional Concepts, J_c

```
C
C     ============================================================
C
C     MAIN PROGRAM FOR CALCULATING THE ELECTRIC CURRENT IN A
C     P-TYPE SHOTTKY BARRIER
C
C     USEAGE: REQUIRES THE SUBROUTINES
C             SUBROUTINE ROOT
C             FUNCTION ZERO
C             SUBROUTINE XFERMI
C             FUNCTION EFERMI
C             SUBROUTINE QUAD1
C             FUNCTION DIST
C             FUNCTION XINT
C             FUNCTION YINT
C
C
C              TEMP=START OF 1/T TEMP. STEPPING
C              TDLT=TEMP STEP SIZE
C              JMAX=NUMBER OF TEMP STEPS
C              WC=BARRIER HEIGHT FROM TRADITIONAL THEORY
C              WCDLT=STEP SIZE FOR WC
C              IMAX=MAX. NUMBER OF STEPS FOR RATIO
C              EMASS=ELECTRON MASS RATIO (M*/M) FOR METAL
C              SEMASS=ELECTRON MASS RATIO (M*/M) FOR SEMI.
C              FELECT=FREE ELECTRON DENSITY IN METAL
C              VELECT=VALENCE ELECTRON DENSITY IN SEMI.
C
C
C              LUOUT=CHANNEL FOR OUTPUT
C
C
C     ============================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ============================================================
C
      DIMENSION DUMMY(10),A(50),B(50),C(50),D(50),E(50)
      EXTERNAL ZERO,YINT,DIST
```

```
C
C     -----INITIALIZE MISC CONSTANTS-----
C
      XMASS=9.105D-34
      Q=1.61D-19
      BOLTZ=8.61667D-5
      FELECT=1.0D21
      VELECT=1.0D23
      TEMP=3.0D-3
      TDLT=3.0D-3
      JMAX=13
      EMASS=1.0D0
      SEMASS=0.33D0
      WC=0.5D0
      WCDLT=5.0D-2
      IMAX=10
      LUOUT=10
      PI=3.14159265
C
C     -----TOP OF WC STEPPING LOOP-----
C
      DO 40 I=1,IMAX
      WRITE(LUOUT)'WC= ',WC
C
C     -----TOP OF TEMP STEPPING LOOP-----
C
      XTEMP=TEMP
      DO 30 J=1,JMAX
C
      T=1.0D0/XTEMP
C
C     -----CALCULATE FERMI LEVEL-----
C
      CALL XFERMI(FELECT,EF0,T,EMASS,EF,LUOUT)
C
      RATIO=1.0D0-WC/(EF*BOLTZ*T)
C
C     ----CALC SILICON FERMI LEVEL AT ZERO DEG K-----
C
      SEF0=3.0D0*VELECT*1.0D-21/(SEMASS**(3.0D0/2.0D0)*1.2368D1)
      SEF0=SEF0**(2.0D0/3.0D0)
```

```
      SEF0=SEF0/(8.67D-5*T)
C
C     -----CALC DENSITY OF UNOCCUPIED STATES IN VALENCE BAND-----
C
      IEXIT=0
      SUM=0.0D0
      XX=SEF0+EF*(1.0D0-RATIO)
      XUBND=1.0D0-1.0D2/XX
      IF(XUBND.LT.0.0D0) XUBND=0.0D0
      EC=SEF0
   25 CONTINUE
      IF(IEXIT.EQ.1) GOTO 27
      XLBND=XUBND
      XUBND=XUBND+1.0D1/XX
      IF(XUBND.GT.EC/XX) IEXIT=1
      IF(IEXIT.EQ.1) XUBND=EC/XX
      DUMMY(1)=XX
      CALL QUAD1(DIST,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      IF(SUM.LT.1.0D-60) SUM=1.0D-60
      GOTO 25
C
   27 CONTINUE
      YY=3.0D0/2.0D0
      XNV=DLOG(3.0D0/2.0D0)+DLOG(VELECT)-YY*DLOG(SEF0/XX)
      XNV=XNV+DLOG(SUM)
      IF(XNV.LT.-1.6D2) XNV=-1.6D2
      XNV=DEXP(XNV)
      P=SEF0*BOLTZ*T
C     WRITE(10,1122) P,XNV
 1122 FORMAT(1X, 'SEF0=',1PD11.4,3X,'XNV=',1PD11.4)
C
C
C     -----CALC.ET-----
      ET=0.0D0
      IF(RATIO.LT.0.0D0) GOTO 5
C
      DUMMY(1)=FELECT
      DUMMY(3)=EF
      DUMMY(6)=XNV
      DUMMY(7)=T
C
```

```
      ARG=EF*RATIO
      XX=ZERO(ARG,DUMMY)
      IF(XX.GE.0.0D0) ET=ARG
      IF(XX.GE.0.0D0) GOTO 5
C
      ARG=1.0D-25
      XX=ZERO(ARG,DUMMY)
      IF(XX.GE.0.0D0) ET=ARG
      IF(XX.GE.0.0D0) GOTO 5
C
      ET=0.0D0
      ETMAX=1.0D2*EF
      DLTE=EF/1.0D2
      EPS=1.0D-4
C
      CALL ROOT(ZERO,ET,ETMAX,DLTE,EPS,0,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT,'ROOT FOR ET NOT FOUND'
      IF(IER.NE.1) STOP
C
    5 CONTINUE
C
C     -----CALC. CURRENT ABOVE ET-----
C
      XX=ET-EF*RATIO
      XJ1=DLOG(Q)+DLOG(XNV)+DLOG(DSQRT(1.0D0/SEMASS))
      XJ1=XJ1+DLOG(DSQRT(BOLTZ*T/(XMASS*2.0D0*PI)))-XX
      IF(XJ1.LT.-1.6D2) XJ1=-1.6D2
      XJ1=DEXP(XJ1)
C
C     -----CALC. CURRENT BELOW ET-----
C
      SUM=0.0D0
C
      DUMMY(2)=EF
      IEXIT=0
      XUBND=0.0D0
      XX=1.0D0-1.5D2/EF
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      IF(IEXIT.EQ.1) GOTO 20
      XLBND=XUBND
      XUBND=XUBND+1.0D0
```

```
      IF(XUBND.GE.ET) IEXIT=1
      IF(IEXIT.EQ.1) XUBND=ET
      DUMMY(1)=EF
      IF(XUBND-XLBND.LT.1.0D-50) GOTO 15
      CALL QUAD1(YINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
   15 CONTINUE
      GOTO 10
C
      IF(SUM.LT.1.0D-60) SUM=1.6D-60
C
   20 CONTINUE
      XJ2=DLOG(3.0D0)+DLOG(FELECT)-3.0D0*DLOG(EF0)/2.0D0-DLOG(DSQRT(XMASS))
      XJ2=XJ2+DLOG(SUM)+DLOG(DSQRT(1.0D0/EMASS))+DLOG(Q)
      IF(XJ2.LT.-1.6D2) XJ2=-1.6D2
      XJ2=DEXP(XJ2)
C
C     -----CALC. CURRENT USING CONVENTIONAL THEORY-----
C
      XJC=DLOG(Q)+DLOG(XNV)+DLOG(DSQRT(1.0D0/SEMASS))
      XJC=XJC+DLOG(DSQRT(BOLTZ*T/(2.0D0*PI*XMASS)))-EF*(1.0D0-RATIO)
      IF(XJC.LT.-1.6D2) XJC=-1.6D2
      XJC=DEXP(XJC)
C
C     -----STORE RESULTS-----
C
      A(J)=DLOG10(XJ1)
      B(J)=1.0D0/T
      C(J)=DLOG10(XJ2)
      D(J)=DLOG10(XJC)
      E(J)=DLOG10(XJ1+XJ2)
      EB=EF*RATIO*BOLTZ*T
      EF=EF*BOLTZ*T
      EF0=EF0*BOLTZ*T
      ET=ET*BOLTZ*T
      WRITE(LUOUT,1111) EF,EB,T,ET,XJ1,XJ2,XJC
 1111 FORMAT(1X,'EF=',1PD12.5,3X,'EB=',1PD12.5,3X,'TEMP=',1PD10.3,
     &3X,'ET=',1PD12.5,3X,'XJ1=',1PD12.5,3X,'XJ2=',1PD12.5,3X,'XJC='
     &,1PD12.5)
C
      XTEMP=XTEMP+TDLT
   30 CONTINUE
```

```
      WRITE(LUOUT)
C
C
      WD=WD-WCDLT
   40 CONTINUE
      END
```

```
C
C
C     ================================== ==============================
C
C     SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
C
C     USAGE  :   CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     WHERE  :   B(X,DUMMY)  =  ARBITRARY FUNCTION
C
C     .          DUMMY       =  A 10 ELEMENT ARRAY USED FOR PASSING
C     .                         PARAMETERS TO THE FUNCTION "B"
C
C     .          X           =  MIN (MAX) VALUE OF X BEGINING SEARCH
C
C     .          XMAX        =  MAX (MIN) VALUE OF X DURING SEARCH
C
C     .          DELX        =  INITIAL STEP SIZE
C     .                         ( +DELX INCREASES X , -DELX DECREASES X )
C
C     .          EPS         =  PERMITTED FRACTIONAL ERROR
C
C     .          IAR         =  ITERATION METHOD
C     .                         ( IAR = 0  BINARY CHOP )
C     .                         ( IAR = 1  METHOD OF SECANTS )
C
C     .          IER         =  ERROR FLAG
C     .                         ( IER = 1 ROOT FOUND )
C     .                         ( IER = 0 ROOT NOT FOUND )
C
C     COMMENT :  THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
C     .          PROGRAM MUST CLASSIFY THE FUNCTION NAME
C     .          TO BE PASSED THROUGH "B" AS EXTERNAL.
C
C     ================================================================
C     ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
C
C     MOD#1    : AERC  C.L. KENNEDY   NOV. 1978
C     .                  IF X REACHES XMAX SET X=0 AND RETURN
C
```

```
C     MOD#2    : AERC  D.P. KENNEDY NOV 1978
C     .                    INTRODUCED ERROR FLAG IER
C
C     MOD#3    : AERC  D.P. KENNEDY  NOV. 1978
C     .                    EPS=FRACTIONAL CHANGE IN X
C     .                    METHOD OF SECANTS INTRODUCED
C
C     MOD#4    : AERC  C.L. KENNEDY DECEMBER 1978
C     .                    ALL DUMMY VARIABLES PASSED
C     .                    THROUGH ARRAY DUMMY
C
C     ================================================================
C
C
      SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     #      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION P(2),Q(2),DUMMY(1)
C
      IF (DELX.EQ.0.0D0) GOTO 90
      IER=1
      P(1)=0.0D0
      P(2)=0.0D0
      Q(1)=0.0D0
      Q(2)=0.0D0
      Y=B(X,DUMMY)
      P(1)=X
C
C     ----------------------------------------------------------------
C     S T E P    T O    B R A C K E T    R O O T
C     ----------------------------------------------------------------
C
   10 X=X+DELX
      P(2)=X
      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
```

```
      IF(A.LT.0.0D0) GOTO 15
      Y=Z
      GOTO 10
C
C     ------------------------------------------------------------------
C     B I N A R Y   C H O P   O R   M E T H O D   O F   S E C A N T S ?
C     ------------------------------------------------------------------
C
   15 DEL=DELX
      IF(IAR.EQ.1) GOTO 60
C
C     ------------------------------------------------------------------
C     B I N A R Y   C H O P
C     ------------------------------------------------------------------
C
   20 Y=Z
      P(1)=P(2)
   30 DEL=DEL/2.0D0
      X=X-DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 40
      GOTO 30
C
   40 Y=Z
      P(1)=P(2)
   50 DEL=DEL/2.0D0
      X=X+DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 20
      GOTO 50
C
C     ------------------------------------------------------------------
```

```
C     M E T H O D   O F   S E C A N T S
C     ------------------------------------------------------------
C
   60 Q(2)=Z
      P(2)=X
      P(1)=X-DEL
      PREP=P(1)
      Q(1)=B(DUMMY,PREP)
   70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
      YY=B(XX,DUMMY)
      P(1)=P(2)
      Q(1)=Q(2)
      P(2)=XX
      Q(2)=YY
      ERROR=DABS((P(1)-P(2))/P(2))
      IF(ERROR.LE.EPS) GOTO 80
      GOTO 70
   80 X=XX
      RETURN
C
C     ------------------------------------------------------------
C     E R R O R   R E T U R N   X = 0   I E R = 0
C     ------------------------------------------------------------
C
   90 X=0.0D0
      IER=0
      RETURN
      END
```

```
C
C     ================================================
C     FUNCTION ZERO: CALCULATES WITHIN AN ENERGY RANGE E AND
C                    (E+DE) THE DIFFERENCE BETWEEN UNOCCUPIED
C                    STATES IN THE METAL AND ELECTRONS WITH
C                    A MAXWELLIAN DISTRIBUTION THAT ARE
C                    AVAILABLE TO OCCUPY THESE STATES
C
C     ================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE, FLA.
C
C     ================================================
C
      FUNCTION ZERO(ARG,DUMMY)
      DIMENSION DUMMY(10)
      FELECT=DUMMY(1)
      EF=DUMMY(3)
      XNV=DUMMY(6)
      T=DUMMY(7)
      BOLTZ=8.61666D0
      PI=3.14159265
C
C
      XX=ARG
      IF(DABS(XX).LE.1.0D-70) XX=1.0D-70
      TERM1=DLOG(3.0D0)+DLOG(FELECT)-3.0D0*DLOG(EF0)/2.0D0+DLOG(XX)
      XX=EF-ARG
      IF(XX.GT.1.5D2) TERM1=TERM1-XX
      IF(XX.GT.1.5D2) GOTO 10
      IF(XX.LT.-1.5D2) GOTO 10
      TERM1=TERM1-DLOG(1.0D0+DEXP(XX))
   10 CONTINUE
C
C
      TERM2=-DLOG(DSQRT(1.0D0/(2.0D0*PI*BOLTZ*T)))+DLOG(XNV)
      XX=ARG-RATIO*EF
      TERM2=TERM2-XX

      ZERO=TERM1-TERM2
```

```
C
      RETURN
      END
```

```
      COMPILER DOUBLE PRECISION
C
C     ================================================================
C
C     SUBROUTINE XFERMI IS USED TO CALCULATE  THE FERMI LEVEL
C                     IN A METAL AT A SPECIFIED TEMP
C
C     USEAGE: REQUIRES THE FOLLOWING
C             FUNCTION EFERMI
C             SUBROUTINE ROOT
C             FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC.. GAINESVILLE FLA.
C
C     ================================================================
C
      SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUOUT)
C
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL EFERMI
C
C
C
C     -----CALCULATE FERMI LEVEL AT ZERO K-----
C
      EF0=3.0D0*ELECT*1.0D-21/(EMASS**(3.0D0/2.0D0)*1.2368D1)
      EF0=EF0**(2.0D0/3.0D0)
      EF0=EF0/(8.617D-5*T)
C
C     -----CALCULATE FERMI LEVEL-----
C
      DUMMY(1)=EF0
      EF=EF0*0.75D0
      EFMAX=1.0D2*EF0
      DELTE=EF0*5.0D-1
      EPS=1.0D-4
C
```

```
      CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND
      IF(IER.NE.1) STOP
      END
```

```
C     ================================================================
C     SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
C                       LEGENDRE TYPE
C
C
C     USEAGE: CALL QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C             FUNC   =FUNCTION TO BE INTEGRATED. THIS FUNCTION
C                     MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
C             DUMMY  = 1-DIM DUMMY ARRAY FOR PASSING DATA
C                      TO FUNC. THIS ARRAY MUST BE DIMENTIONED
C                      IN THE CALLING PROGRAM.
C .           XLBND  = LOWER BOUND OF THE INTEGRAL
C .           XUBND  = UPPER BOUND OF THE INTEGRAL
C .           RES    = RESULT
C             IAR    = NUMBER OF TERMS IN THE INTEGRATION
C                      (MAX=16,MIN=2)
C
C
C       NOTE:
C .          FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
C .               CALLING PROGRAM
C
C
C     REFERENCE:
C .         NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
C .              CHAPMAN HALL, LONDON, 1961
C
C
C     ================================================================
C     ORIGIONAL:C.L. KENNEDY OCT. 1978
C                  C.L. KENNEDY
C       MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
C             TO 16 TERMS  SEPT 1981
C     ================================================================
C
C
      SUBROUTINE QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C
C
      COMMON /QUAD/ Z(8,16),W(8,16)
```

```
      DIMENSION DUMM(1)
C
      DATA Z / 8*0.0D0,
     &.57735026918962GD0,7*0.0D0,
     $0.774596669241483D0,7*0.0D0,
     $0.861136311594053D0,0.339981043584856D0,6*0.0D0,
     $0.906179845938664D0,0.538469310105683D0,6*0.0D0,
     $0.932469514203152D0,0.661209386466265D0,0.238619186083197D0,5*0.0D0,
     $0.949107912342759D0,0.741531185599394D0,0.405845151377397D0,5*0.0D0,
     $0.960289856497536D0,0.796666477413627D0,0.525532409916329D0,
     $0.183434642495650D0,4*0.0D0,
     $0.968160239507626D0,0.836031107326636D0,0.613371432700590D0,
     $0.324253423403809D0,4*0.0D0,
     $0.973906528517172D0,0.865063366688985D0,0.679409568299024D0,
     $0.433395394129247D0,0.148874338981631D0,3*0.0D0,
     $0.978228658146057D0,0.887062599768095D0,0.730152005574049D0,
     $0.519096129206812D0,0.269543155952345D0,3*0.0D0,
     $0.981560634246719D0,0.904117256370475D0,0.769902674194305D0,
     $0.587317954286617D0,0.367831498998180D0,0.125233408511469D0,
     $2*0.0D0,
     $0.984183054718588D0,0.917598399222978D0,0.801578090733310D0,
     $0.642349339440340D0,0.448492751036447D0,0.230458315955135D0,
     $2*0.0D0,
     $0.986283808696812D0,0.928434883663574D0,0.827201315069765D0,
     $0.687292904811685D0,0.515248636358154D0,0.319112368927890D0,
     $0.108054948707344D0,0.0D0,
     $0.987992518020485D0,0.937273924007060,0.848206583410427D0,
     $0.724417731360170D0,0.570972172608539D0,0.394151347077563D0,
     $0.201194093997435D0,0.0D0,
     $0.989400934991650D0,0.944575023073233D0,0.865631202387832D0,
     $0.755404408355003D0,0.617876244402644D0,0.458016777657227D0,
     $0.281603550779259D0,0.095012509837637D0/
C
      DATA W / 8*0.0D0,
     $1.0D0,7*0.0D0,
     $0.555555555555556D0,0.888888888888889D0,6*0.0D0,
     $0.347854845137454D0,0.652145154862546D0,6*0.0D0,
     $0.236926885056189D0,0.478628670499366D0,0.568888888888889D0,
     $5*0.0D0,0.171324492379170D0,0.360761573048139D0,
     $0.467913934572691D0,5*0.0D0,0.129484966168870D0,
     $0.279705391489277D0,0.381830050505119D0,0.417959183673469D0,
     $4*0.0D0,0.101228563290376D0,0.222381034453374D0,
```

```
     $0.313706645877887D0,0.362683783378362D0,
     $4*0.0D0,0.031274389315740D0,0.130648160632957D0,
     $0.260106964029350D0,0.312347077240003D0,0.330239355301260D0,
     $3*0.0D0,0.066571344308688D0,0.149451349150581D0,
     $0.219086362515982D0,0.269266719309996D0,0.295524224714753D0,
     $3*0.0D0,0.055668567116174D0,0.125580369464905D0,
     $0.186290210927734D0,0.233193764591990D0,
     $0.262804544510247D0,0.272925086777901D0,2*0.0D0,
     $0.047175336386512D0,0.106939325995318D0,0.160078328543346D0,
     $0.203167426723066D0,0.233492536538355D0,0.249147045813403D0,
     $2*0.0D0,0.040484004765316D0,0.092121499837728D0,
     $0.138873510219787D0,0.178145980761946D0,0.207816047536888D0,
     $0.226283180262897D0,0.232551553230874D0,0.0D0,
     $0.035119460331752D0,0.080158087159760D0,0.121518570687903D0,
     $0.157203167158194D0,0.185538397477938D0,0.205198463721296D0,
     $0.215263853463158D0,0.0D0,0.030753241996117D0,
     $0.070366047488108D0,0.107159220467172D0,0.139570677926154D0,
     $0.166269205816994D0,0.186161000015562D0,0.198431485327112D0,
     $0.202578241925561D0,0.027152459411754D0,0.062253523938648D0,
     $0.095158511682493D0,0.124628971255534D0,0.149595988816577D0,
     $0.169156519395003D0,0.182603415044924D0,0.189450610455068D0/
C
C
C
      SUM=0.0D0
      DO 10 I=1,8
      IF(W(I,IAR).EQ.0) GOTO 10
      ARG=(Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
      ARG=(-Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM2=0.0D0
      IF(Z(I,IAR).NE.0.0D0) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
      SUM=SUM+TERM1+TERM2
   10 CONTINUE
C
      RES=SUM*(XUBND-XLBND)/2.0D0
C
      RETURN
      END
```

```
      FUNCTION DIST(ARG,DUMMY)
C
C     ========== ================================================
C
C     FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   UNOCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EFC=DUMMY(1)
C
      A=DSQRT(ARG)
      B=EFC*(1.0D0-ARG)
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      DIST=A/DENOM
C
C
      RETURN
      END
```

```
      FUNCTION XINT(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION XINT:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   OCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
C
      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      XINT=A/DENOM
C
C
      RETURN
      END
```

```
      FUNCTION YINT(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION YINT IS THE INTEGRAND FOR CALCULATING THE
C                   ELECTRIC CURRENT IN A P-TYPE SCHOTTKY
C                   BARRIER IN THE REGION BELOW ET
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE FLA.
C
C     ================================================================
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
C
      IF(ARG.GT.1.6D2) ARG=1.6D2
      IF(ARG.LT.-1.6D2) ARG=-1.6D2
      A=DLOG(ARG)
      B=EF-ARG
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=(1.0D0+DEXP(B))
      IF(DENOM.GT.1.0D70) DENOM=1.0D70
      IF(DENOM.LT.-1.0D70) DENOM=-1.0D70
      DENOM=DLOG(DENOM)
      YINT=A-B
      IF(YINT.GT.1.6D2) YINT=1.6D2
      IF(YINT.LT.-1.6D2) YINT=-1.6D2
      YINT=DEXP(YINT)
C
C
      RETURN
      END
```

```
C
C     ================================================================
C
C     FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
C                      METALLIC CONDUCTOR
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      FUNCTION EFERMI(EF,DUMMY)
      DIMENSION DUMMY(10)
      EXTERNAL XINT
C
C     -----INTEGRATE FROM 0 TO INF-----
C
      EF0=DUMMY(1)
      DUMMY(2)=EF
      SUM=0.0D0
      XX=EF-1.2D1
      IF(XX.GT.0.0D0) SUM=2.0D0*(XX**(3.0D0/2.0D0))/3.0D0
      XUBND=0.0D0
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      XLBND=XUBND
      XUBND=XUBND+1.0D1
      XX=XUBND-EF
      IF(XX.GT.1.0D2) GOTO 30
      CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   30 CONTINUE
      EFERMI=1.0D0-3.0D0*EF0**(-3.0D0/2.0D0)*SUM/2.0D0
C
C
```

```
      RETURN
      END
```

APPENDIX I-G

Program for Calculating the Volt-Ampere Characteristics of a Schottky Barrier Based Upon the Concepts Developed During This Research, and Upon Traditional Concepts of Device Operation

```
C
C     ================================================================
C
C     MAIN PROGRAM FOR CALCULATION OF CURRENT/VOLTAGE CURVES
C     FOR A P-TYPE SCHOTTKY BARRIER
C
C     USEAGE: REQUIRES THE SUBROUTINES
C             SUBROUTINE ROOT
C             FUNCTION ZERO
C             SUBROUTINE XFERMI
C             SUBROUTINE QUAD1
C             SUBROUTINE XTEMPR
C             FUNCTION DIST
C             FUNCTION XINT
C             FUNCTION YINT
C             FUNCTION EQU
C
C
C              ACCPTR=ACCEPTOR DENSITY IN SILICON
C              TEMP=TEMPERATURE OF DEVICE OPERATION
C              BARRER=BARRIER HEIGHT FROM TRADITIONAL THEORY
C              WCDLT=STEP SIZE FOR BARRIER HEIGHT
C              IMAX=NUMBER OF STEPS FOR WC
C              EMASS=ELECTRON MASS RATIO (M*/M) FOR METAL
C              SEMASS=ELECTRON MASS RATIO (M*/M) FOR SEMI.
C              FELECT=FREE ELECTRON DENSITY IN METAL
C              DLTNC=STEP SIZE FOR FELECT
C              LMAX=NUMBER OF FELECT STEPS
C              VELECT=VALENCE ELECTRON DENSITY IN SEMI.
C              VAPPL=START OF APPLIED VOLTAGE STEPPING
C              VDLT =SIZE OF STEP FOR VAPPL
C              JMAX=NUMBER OF VAPPL STEPS
C
C
C              LUOUT=CHANNEL FOR OUTPUT
C
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
```

```
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EXTERNAL ZERO,YINT,DIST
C
C     -----INITIALIZE MISC CONSTANTS-----
C

      ACCPTR=1.5D15
      VAPPL=0.0D0
      VDLT=0.1D0
      JMAX=21
      XMASS=9.105D-34
      Q=1.61D-19
      BOLTZ=8.61667D-5
      FELECT=1.0D20
      DLTNC=1.0D19
      LMAX=6
      VELECT=1.0D23
      TEMP=7.7D1
      EMASS=1.0D0
      SEMASS=0.33D0
      BARRER=2.7D-1
      WCDLT=5.0D-2
      IMAX=1
      LUOUT=10
      PI=3.14159265
      EPS=8.86D-14
      DIELK=11.7
      T=TEMP
C
C     -----TOP OF NC STEPPING LOOP-----
C
      XNC=FELECT
      DO 50 L=1,LMAX
      WRITE(LUOUT)'XNC=',XNC
C
C     -----TOP OF WC STEPPING LOOP-----
C
      WC=BARRER
      DO 40 I=1,IMAX
```

```
C
C     -----TOP OF VOLTAGE STEPPING LOOP-----
C
      XV=VAPPL
      DO 30 J=1,JMAX
C
C     -----CALCULATE FERMI LEVEL-----
C
      CALL XFERMI(XNC,EF0,T,EMASS,EF,LUOUT)
C
C
C     -----CALC ION DENSITY AND VDIFF IN DEVICE-----
C
      XB=BOLTZ*3.0D2
      CALL XTEMPR(XION,ENSUBI,VDIFF,EIF,EIV,T,HOLES,EGAP,XB,ACCPTR,
     $WC,LUOUT)
      V=XV+VDIFF
C
C     -----CALCULATE SPACE CHARGE ELECTRIC FIELD-----
C
      FIELD=DSQRT(Q*XION*V/(DIELK*EPS))
      XWC=WC-3.79D-4*DSQRT(FIELD)
      RATIO=1.0D0-XWC/(EF*BOLTZ*T)
C
C     ----CALC SILICON FERMI LEVEL AT ZERO DEG K-----
C
      SEF0=3.0D0*VELECT*1.0D-21/(SEMASS**(3.0D0/2.0D0)*1.2368D1)
      SEF0=SEF0**(2.0D0/3.0D0)
      SEF0=SEF0/(8.67D-5*T)
C
C     -----CALC DENSITY OF UNOCCUPIED STATES IN VALENCE BAND-----
C
      IEXIT=0
      SUM=0.0D0
      XX=SEF0+EF*(1.0D0-RATIO)
      XUBND=1.0D0-1.0D2/XX
      IF(XUBND.LT.0.0D0) XUBND=0.0D0
      EC=SEF0
   25 CONTINUE
      IF(IEXIT.EQ.1) GOTO 27
      XLBND=XUBND
      XUBND=XUBND+1.0D1/XX
```

```
      IF(XUBND.GT.EC/XX) IEXIT=1
      IF(IEXIT.EQ.1) XUBND=EC/XX
      DUMMY(1)=XX
      CALL QUAD1(DIST,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      IF(SUM.LT.1.0D-60) SUM=1.0D-60
      GOTO 25
C
   27 CONTINUE
      YY=3.0D0/2.0D0
      XNV=DLOG(3.0D0/2.0D0)+DLOG(VELECT)-YY*DLOG(SEF0/XX)
      XNV=XNV+DLOG(SUM)
      IF(XNV.LT.-1.6D2) XNV=-1.6D2
      XNV=DEXP(XNV)
C
C     -----CALC.ET-----
C
      ET=0.0D0
      IF(RATIO.LT.0.0D0) GOTO 5
C
      DUMMY(1)=XNC
      DUMMY(3)=EF
      DUMMY(6)=XNV
      DUMMY(7)=T
C
      ARG=EF*RATIO
      XX=ZERO(ARG,DUMMY)
      IF(XX.GE.0.0D0) ET=ARG
      IF(XX.GE.0.0D0) GOTO 5
C
      ARG=1.0D-25
      XX=ZERO(ARG,DUMMY)
      IF(XX.GE.0.0D0) ET=ARG
      IF(XX.GE.0.0D0) GOTO 5
C
      ET=0.0D0
      ETMAX=1.0D2*EF
      DLTE=EF/1.0D2
      EPS=1.0D-4
C
      CALL ROOT(ZERO,ET,ETMAX,DLTE,EPS,0,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT,'ROOT FOR ET NOT FOUND'
```

```
      IF(IER.NE.1) STOP

    5 CONTINUE
C
C     -----CALC. CURRENT ABOVE ET-----
C
      XX=ET-EF*RATIO
      XJ1=DLOG(Q)+DLOG(XNV)+DLOG(DSQRT(1.0D0/SEMASS))
      XJ1=XJ1+DLOG(DSQRT(BOLTZ*T/(XMASS*2.0D0*PI)))-XX
      IF(XJ1.LT.-1.6D2) XJ1=-1.6D2
      XJ1=DEXP(XJ1)
C
C     -----CALC. CURRENT BELOW ET-----
C
      SUM=0.0D0
C
      DUMMY(2)=EF
      IEXIT=0
      XUBND=0.0D0
      XX=1.0D0-1.5D2/EF
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      IF(IEXIT.EQ.1) GOTO 20
      XLBND=XUBND
      XUBND=XUBND+1.0D0
      IF(XUBND.GE.ET) IEXIT=1
      IF(IEXIT.EQ.1) XUBND=ET
      DUMMY(1)=EF
      IF(XUBND-XLBND.LT.1.0D-50) GOTO 15
      CALL QUAD1(YINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
   15 CONTINUE
      GOTO 10
C
      IF(SUM.LT.1.0D-60) SUM=1.6D-60
C
   20 CONTINUE
      XJ2=DLOG(3.0D0)+DLOG(XNC)-3.0D0*DLOG(EF0)/2.0D0-DLOG(DSQRT(XMASS))
      XJ2=XJ2+DLOG(SUM)+DLOG(DSQRT(1.0D0/EMASS))+DLOG(Q)
      IF(XJ2.LT.-1.6D2) XJ2=-1.6D2
      XJ2=DEXP(XJ2)
C
```

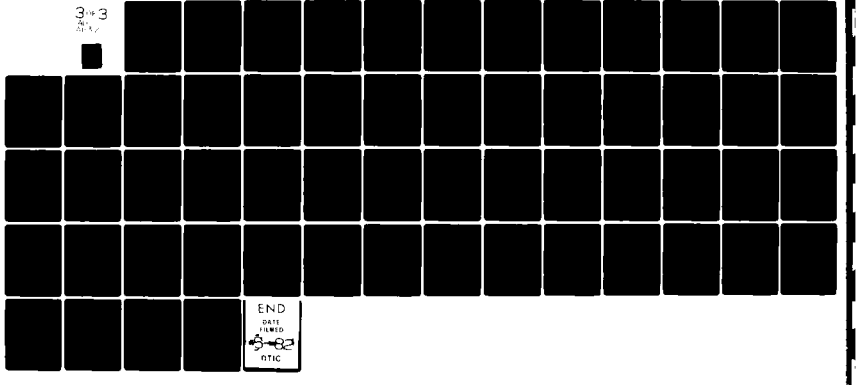
```
C     -----CALC. CURRENT USING CONVENTIONAL THEORY-----
C
      XJC=DLOG(Q)+DLOG(XNV)+DLOG(DSQRT(1.ØDØ/5EMASS))
      XJC=XJC+DLOG(DSQRT(BOLTZ*T/(2.ØDØ*PI*XMASS)))-EF*(1.ØDØ-RATIO)
      IF(XJC.LT.-1.6D2) XJC=-1.6D2
      XJC=DEXP(XJC)
C
C     -----PRINT RESULTS-----
C
      XJT=XJ1+XJ2
      XJT=DLOG(XJT)
      XX=XV/(BOLTZ*T)
      IF(XX.GT.1.6D2) XX=1.6D2
      XX=1.ØDØ-DEXP(-XX)
      IF(XX.LT.1.ØD-7Ø) XX=1.ØD-7Ø
      XX=DLOG(XX)
      XJT=XJT+XX
      IF(XJT.GT.1.6D2) XJT=1.6D2
      IF(XJT.LT.-1.6D2) XJT=-1.6D2
      XJT=DEXP(XJT)
C
      XJC=DLOG(XJC)
      XJC=XJC+XX
      IF(XJC.GT.1.6D2) XJC=1.6D2
      IF(XJC.LT.-1.6D2) XJC=-1.6D2
      XJC=DEXP(XJC)
C
      EB=EF*RATIO*BOLTZ*T
      EF=EF*BOLTZ*T
      EFØ=EFØ*BOLTZ*T
      ET=ET*BOLTZ*T
C
      WRITE(LUOUT,1ØØØ) EF,EB,XV,ET
      WRITE(LUOUT,1Ø1Ø) XJ1,XJ2,XJC,XJT
 1ØØØ FORMAT(1X,'EF=',1PD12.5,3X,'EB=',1PD12.5,3X,'VAPPL=',1PD12.5.
     &3X,'ET=',1PD12.5)
 1Ø1Ø FORMAT(1X,'XJ1=',1PD12.5,3X,'XJ2=',1PD12.5,3X,'XJC=',1PD12.5
     &,3X,'XJT=',1PD12.5,/)
C
      XV=XV+VDLT
   3Ø CONTINUE
      WC=WC-WCDLT
```

```
C
   40 CONTINUE
      XNC=XNC+DLTNC
   50 CONTINUE
      END
```

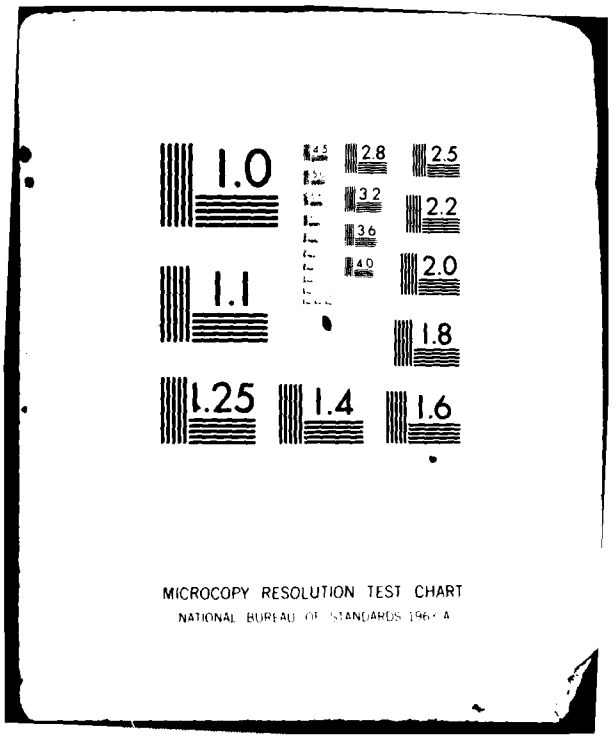
```
C
C     ================================================================
C
C     SUBROUTINE XTEMPR:IS USED TO CALCULATE MANY TEMP DEPENDENT
C                       PROPERTIES OF SILICON, IN ADDITION TO THE
C                       DIFF POTENTIAL OF A PT-SI BARRIER
C
C                       XION=IONIZED BORON ATOMS (CM**-3)
C                       ENSUBI=NI (CM**-3)
C                       VDIFF=DIFF POTENTIAL (VOLTS)
C                       EIF=EI-EF IN EV
C                       EIV=EI-EV IN EV
C                       TEMP=TEMPERATURE  DEG.K
C                       HOLES=HOLE DENSITY (CM**-3)
C                       EGAP=ENERGY GAP IN EV
C                       ACCPTR=ACCPTR DENSITY (CM**-3)
C                       BARRER=ENERGY BARRIER (EV) FOR VDIFF CALC
C                       BOLTZ=BOLTZMANN CONSTANT AT 300 DEG. K
C
C                       LUOUT=OUTPUT CHANNEL
C
C     USEAGE: REQUIRES SUBROUTINE ROOT AND FUNCTION EQU
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.
C
C     ================================================================
C
      SUBROUTINE XTEMPR(XION,ENSUBI,VDIFF,EIF,EIV,TEMP,HOLES,EGAP,BOLTZ,
     &ACCPTR,BRRIER,LUOUT)
      DIMENSION DUMMY (11)
      EXTERNAL EQU
C
C
      T=TEMP/3.D2
      EGAP=1.165-7.242D-3*T-3.664D-2*T*T
      EIV=EGAP/2.D0-1.306D-2*T
      ENSUBI=3.925D19*T*DSQRT(T)*DEXP(-EGAP/(2.0D0*BOLTZ*T))
```

AD-A113 211 KENNEDY (D P) AND ASSOCIATES INC GAINESVILLE FL F/G 20/12
INVESTIGATION OF THE CURRENT VOLTAGE RELATIONSHIP FOR LOW BARRI--ETC(U)
FEB 82 D P KENNEDY F19628-80-C-0020

UNCLASSIFIED RADC-TR-82-13 NL



END
DATE FILMED
5-82
DTIC


1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS 1963-A

```
C
C
      DUMMY(1)=EGAP
      DUMMY(2)=EIV
      DUMMY(3)=ENSUBI
      DUMMY(4)=T
      DUMMY(5)=BOLTZ
      DUMMY(6)=BRRIER
      DUMMY(7)=ACCPTR
C
      EIF=EIV
      EIFMX=-EIV
      DLTEI=-EIV/2.ØD1
C
      CALL ROOT(EQU,EIF,EIFMX,DLTEI,1.ØD-6,Ø,IER,DUMMY)
C
      IF(IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND IN XTEMPR'
C
      XION=DUMMY(8)
      EAF=DUMMY(9)
      EFV=DUMMY(1Ø)
      HOLES=DUMMY(11)
C
      VDIFF=BRRIER-EFV
C
      RETURN
      END
```

```
      FUNCTION EQU(EIF,DUMMY)
C
      DIMENSION DUMMY(11)
C
      EGAP=DUMMY(1)
      EIV=DUMMY(2)
      ENSUBI=DUMMY(3)
      T=DUMMY(4)
      BOLTZ=DUMMY(5)
      BRRIER=DUMMY(6)
      ACCPTR=DUMMY(7)
C
      EFV=EIV-EIF
      EAF=4.38D-2-3.037D-8*ACCPTR**(1.0/3.0)-EFV
      XION=1.0D0/(1.0+(4.0+2.0/DEXP(4.4D-2/(BOLTZ*T)))*DEXP(EAF/(BOLTZ*T)))
      XION=XION*ACCPTR
C
      HOLES=ENSUBI*DEXP(EIF/(BOLTZ*T))
      EQU=(HOLES-XION)/ACCPTR
C
      DUMMY(8)=XION
      DUMMY(9)=EAF
      DUMMY(10)=EFV
      DUMMY(11)=HOLES
C
      RETURN
      END
```

```
C
C
C     ================================================================
C
C     SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
C
C     USAGE  :   CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     WHERE  :   B(X,DUMMY)  =  ARBITRARY FUNCTION
C
C     .          DUMMY       =  A 10 ELEMENT ARRAY USED FOR PASSING
C     .                         PARAMETERS TO THE FUNCTION "B"
C
C     .          X           =  (MAX) VALUE OF X BEGINING SEARCH
C
C     .          XMAX        =  MAX (MIN) VALUE OF X DURING SEARCH
C
C     .          DELX        =  INITIAL STEP SIZE
C     .                         ( +DELX INCREASES X , -DELX DECREASES X )
C
C     .          EPS         =  PERMITTED FRACTIONAL ERROR
C
C     .          IAR         =  ITERATION METHOD
C     .                         ( IAR = 0  BINARY CHOP )
C     .                         ( IAR = 1  METHOD OF SECANTS )
C
C     .          IER         =  ERROR FLAG
C     .                         ( IER = 1 ROOT FOUND )
C     .                         ( IER = 0 ROOT NOT FOUND )
C
C     COMMENT :  THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
C     .          PROGRAM MUST CLASSIFY THE FUNCTION NAME
C     .          TO BE PASSED THROUGH "B" AS EXTERNAL.
C
C     ================================================================
C     ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
C
C     MODN1    : AERC  C.L. KENNEDY   NOV. 1978
C     .                  IF X REACHES XMAX SET X=0 AND RETURN
C
```

```
C     MOD#2    : AERC  D.P. KENNEDY NOV 1978
C     .                INTRODUCED ERROR FLAG IER
C
C     MOD#3    : AERC  D.P. KENNEDY  NOV. 1978
C     .                EPS=FRACTIONAL CHANGE IN X
C     .                METHOD OF SECANTS INTRODUCED
C
C     MOD#4    : AERC  C.L. KENNEDY DECEMBER 1978
C     .                ALL DUMMY VARIABLES PASSED
C     .                THROUGH ARRAY DUMMY
C
C     ================================================================
C
C
      SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C
C     #      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION P(2),Q(2),DUMMY(1)
C
      IF (DELX.EQ.0.0D0) GOTO 90
      IER=1
      P(1)=0.0D0
      P(2)=0.0D0
      Q(1)=0.0D0
      Q(2)=0.0D0
      Y=B(X,DUMMY)
      P(1)=X
C
C     ----------------------------------------------------------------
C     S T E P    T O    B R A C K E T    R O O T
C     ----------------------------------------------------------------
C
   10 X=X+DELX
      P(2)=X
      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
```

```
      IF(A.LT.0.0D0) GOTO 15
      Y=Z
      GOTO 10
C
C     ------------------------------------------------------------------
C     B I N A R Y   C H O P   O R   M E T H O D   O F   S E C A N T S ?
C     ------------------------------------------------------------------
C
   15 DEL=DELX
      IF(IAR.EQ.1) GOTO 60
C
C     ------------------------------------------------------------------
C     B I N A R Y    C H O P
C     ------------------------------------------------------------------
C
   20 Y=Z
      P(1)=P(2)
   30 DEL=DEL/2.0D0
      X=X-DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 40
      GOTO 30
C
   40 Y=Z
      P(1)=P(2)
   50 DEL=DEL/2.0D0
      X=X+DEL
      P(2)=X
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF(DABS(AB).LE.EPS) RETURN
      A=Y*Z
      P(1)=P(2)
      IF (A.LT.0.0D0) GOTO 20
      GOTO 50
C
C     ------------------------------------------------------------------
```

```
C     METHOD OF SECANTS
C     -----------------

   60 Q(2)=Z
      P(2)=X
      P(1)=X-DEL
      PREP=P(1)
      Q(1)=B(DUMMY,PREP)
   70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
      YY=B(XX,DUMMY)
      P(1)=P(2)
      Q(1)=Q(2)
      P(2)=XX
      Q(2)=YY
      ERROR=DABS((P(1)-P(2))/P(2))
      IF(ERROR.LE.EPS) GOTO 80
      GOTO 70
   80 X=XX
      RETURN
C
C     ------------------------------------------------------------
C     ERROR   RETURN   X = 0   IER = 0
C     ------------------------------------------------------------
C
   90 X=0.0D0
      IER=0
      RETURN
      END
```

```
C
C     ================================================
C     FUNCTION ZERO: CALCULATES WITHIN AN ENERGY RANGE E AND
C                    (E+DE) THE DIFFERENCE BETWEEN UNOCCUPIED
C                    STATES IN THE METAL AND ELECTRONS WITH
C                    A MAXWELLIAN DISTRIBUTION THAT ARE
C                    AVAILABLE TO OCCUPY THESE STATES
C
C     ================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE, FLA.
C
C     ================================================
C
      FUNCTION ZERO(ARG,DUMMY)
      DIMENSION DUMMY(10)
      FELECT=DUMMY(1)
      EF=DUMMY(3)
      XNV=DUMMY(6)
      T=DUMMY(7)
      BOLTZ=8.61666D0
      PI=3.14159265
C
C
      XX=ARG
      IF(DABS(XX).LE.1.0D-70) XX=1.0D-70
      TERM1=DLOG(3.0D0)+DLOG(FELECT)-3.0D0*DLOG(EF0)/2.0D0+DLOG(XX)
      XX=EF-ARG
      IF(XX.GT.1.5D2) TERM1=TERM1-XX
      IF(XX.GT.1.5D2) GOTO 10
      IF(XX.LT.-1.5D2) GOTO 10
      TERM1=TERM1-DLOG(1.0D0+DEXP(XX))
   10 CONTINUE
C
C
      TERM2=-DLOG(DSQRT(1.0D0/(2.0D0*PI*BOLTZ*T)))+DLOG(XNV)
      XX=ARG-RATIO*EF
      TERM2=TERM2-XX

      ZERO=TERM1-TERM2
```

```
C
      RETURN
      END
```

```
      COMPILER DOUBLE PRECISION
C
C     ================================================================
C
C     SUBROUTINE XFERMI IS USED TO CALCULATE  THE FERMI LEVEL
C                     IN A METAL AT A SPECIFIED TEMP
C
C     USEAGE: REQUIRES THE FOLLOWING
C             FUNCTION EFERMI
C             SUBROUTINE ROOT
C             FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.
C
C     ================================================================
C
      SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUOUT)
C
C
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL EFERMI
C
C
C
C     -----CALCULATE FERMI LEVEL AT ZERO K-----
C
      EF0=3.0D0*ELECT*1.0D-21/(EMASS**(3.0D0/2.0D0)*1.2368D1)
      EF0=EF0**(2.0D0/3.0D0)
      EF0=EF0/(8.617D-5*T)
C
C     -----CALCULATE FERMI LEVEL-----
C
      DUMMY(1)=EF0
      EF=EF0*0.75D0
      EFMAX=1.0D2*EF0
      DELTE=EF0*5.0D-1
      EPS=1.0D-4
C
```

```
      CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
      IF(IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND'
      IF(IER.NE.1) STOP
      END
```

```
C     ================================================================
C     SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
C                       LEGENDRE TYPE
C
C
C     USEAGE: CALL QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C             FUNC   =FUNCTION TO BE INTEGRATED. THIS FUNCTION
C                     MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
C             DUMMY  = 1-DIM DUMMY ARRAY FOR PASSING DATA
C                      TO FUNC. THIS ARRAY MUST BE DIMENTIONED
C                      IN THE CALLING PROGRAM.
C .           XLBND  = LOWER BOUND OF THE INTEGRAL
C .           XUBND  = UPPER BOUND OF THE INTEGRAL
C .           RES    = RESULT
C             IAR    = NUMBER OF TERMS IN THE INTEGRATION
C                      (MAX=16,MIN=2)
C
C
C       NOTE:
C .          FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
C .               CALLING PROGRAM
C
C
C     REFERENCE:
C .         NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
C .              CHAPMAN HALL, LONDON, 1961
C
C
C     ================================================================
C     ORIGIONAL:C.L. KENNEDY OCT. 1978
C                  C.L. KENNEDY
C       MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
C             TO 16 TERMS  SEPT 1981
C     ================================================================
C
C
      SUBROUTINE QUAD1(FUNC,XLBND,XUBND,RES,IAR,DUMMY)
C
C
      COMMON /QUAD/ Z(8,16),W(8,16)
```

```
      DIMENSION DUMMY(1)
C
      DATA Z / 8*0.0D0,
     &.57735026918962D0,7*0.0D0,
     $0.77459666924148 3D0,7*0.0D0,
     $0.86113631159405 3D0,0.33998104358485 6D0,6*0.0D0,
     $0.90617984593866 4D0,0.53846931010568 3D0,6*0.0D0,
     $0.93246951420315 2D0,0.66120938646626 5D0,0.23861918608319 7D0,5*0.0D0,
     $0.94910791234275 9D0,0.74153118559939 4D0,0.40584515137739 7D0,5*0.0D0,
     $0.96028985649753 6D0,0.79666477413627 D0,0.52553240991632 9D0.
     $0.18343464249565 0D0,4*0.0D0,
     $0.96816023950762 6D0,0.83603110732663 6D0,0.61337143270590 D0,
     $0.32425342340380 9D0,4*0.0D0,
     $0.97390652851717 2D0,0.86506336688985 D0,0.67940956829902 4D0,
     $0.43339539412924 7D0,0.14887433898163 1D0,3*0.0D0,
     $0.97822865814605 7D0,0.88706259976809 5D0,0.73015200557404 9D0,
     $0.51909612920681 2D0,0.26954315595234 5D0,3*0.0D0,
     $0.98156063424671 9D0,0.90411725637047 5D0,0.76990267419430 5D0,
     $0.58731795428661 7D0,0.36783149899818 0D0,0.12523340851146 9D0,
     $2*0.0D0,
     $0.98418305471858 8D0,0.91759839922297 8D0,0.80157809073331 0D0,
     $0.64234933944034 0D0,0.44849275103644 7D0,0.23045831595513 5D0,
     $2*0.0D0,
     $0.98628380869681 2D0,0.92843488366357 4D0,0.82720131506976 5D0,
     $0.68729290481168 5D0,0.51524863635815 4D0,0.31911236892789 0D0,
     $0.10805494870734 4D0,0.0D0,
     $0.98799251802048 5D0,0.93727339240070 6D0,0.84820658341042 7D0,
     $0.72441773136017 0D0,0.57097217260853 9D0,0.39415134707756 3D0,
     $0.20119409399743 5D0,0.0D0,
     $0.98940093499165 0D0,0.94457502307323 3D0,0.86563120238783 2D0,
     $0.75540440835500 3D0,0.61787624440264 4D0,0.45801677765722 7D0,
     $0.28160355077925 9D0,0.09501250983763 7D0/
C
      DATA W / 8*0.0D0,
     $1.0D0,7*0.0D0,
     $0.55555555555556 D0,0.88888888888889 D0,6*0.0D0,
     $0.34785484513745 4D0,0.65214515486254 6D0,6*0.0D0,
     $0.23692688505618 9D0,0.47862867049936 6D0,0.56888888888888 9D0,
     $5*0.0D0,0.17132449237917 0D0,0.36076157304813 9D0,
     $0.46791393457269 1D0,5*0.0D0,0.12948496616887 0D0,
     $0.27970539148927 7D0,0.38183005050511 9D0,0.41795918367346 9D0,
     $4*0.0D0,0.10122856329037 6D0,0.22238103445337 4D0,
```

```
     $0.313706645877887D0,0.362683783378362D0,
     $4*0.0D0,0.081274388361574D0,0.180648160694857D0,
     $0.260610696402935D0,0.312347077040003D0,0.330239355001260D0,
     $3*0.0D0,0.066671344308688D0,0.149451349150581D0,
     $0.219086362515982D0,0.269266719309996D0,0.295524224714753D0,
     $3*0.0D0,0.055668567116174D0,0.125580369464905D0,
     $0.186290210927734D0,0.233193764591990D0,
     $0.262804544510247D0,0.272925086777901D0,2*0.0D0,
     $0.047175336386512D0,0.106939325995318D0,0.160078328543346D0,
     $0.203167426723066D0,0.233492536538355D0,0.249147045813403D0,
     $2*0.0D0,0.040484004765316D0,0.092121499837728D0,
     $0.138873510219787D0,0.178145980761946D0,0.207816047536889D0,
     $0.226283180262897D0,0.232551553230874D0,0.0D0,
     $0.035119460331752D0,0.080158087159760D0,0.121518570687903D0,
     $0.157203167158194D0,0.185538397477938D0,0.205198463721296D0,
     $0.215263853463158D0,0.0D0,0.030753241996117D0,
     $0.070366047488108D0,0.107159220467172D0,0.139570677926154D0,
     $0.166269205816994D0,0.186161000015562D0,0.198431485327112D0,
     $0.202578241925561D0,0.027152459411754D0,0.062253523938648D0,
     $0.095158511682493D0,0.124628971255534D0,0.149595988816577D0,
     $0.169156519395003D0,0.182603415044924D0,0.189450610455068D0/
C
C
C
      SUM=0.0D0
      DO 10 I=1,8
      IF(W(I,IAR).EQ.0) GOTO 10
      ARG=(Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
      ARG=(-Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.0D0
      TERM2=0.0D0
      IF(Z(I,IAR).NE.0.0D0) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
      SUM=SUM+TERM1+TERM2
   10 CONTINUE
C
      RES=SUM*(XUBND-XLBND)/2.0D0
C
      RETURN
      END
```

```
      FUNCTION DIST(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   UNOCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EFC=DUMMY(1)
C
      A=DSQRT(ARG)
      B=EFC*(1.0D0-ARG)
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      DIST=A/DENOM
C
C
      RETURN
      END
```

```
      FUNCTION XINT(ARG,DUMMY)
C
C     ================================================================
C
C     FUNCTION XINT:REPRESENTS THE DISTRIBUTION FUNCTION FOR
C                   OCCUPIED ENERGY STATES IN A METAL THAT
C                   RESIDE ABOVE THE CONDUCTION BAND EDGE.
C                   THIS DISTRIBUTION IS BASED UPON THE FERMI
C                   -DIRAC DISTRIBUTION
C
C     ================================================================
C
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
C
      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      XINT=A/DENOM
C
C
      RETURN
      END
```

```
      FUNCTION YINT(ARG,DUMMY)
C
C     ============================================================
C
C     FUNCTION YINT IS THE INTEGRAND FOR CALCULATING THE
C                   ELECTRIC CURRENT IN A P-TYPE SCHOTTKY
C                   BARRIER IN THE REGION BELOW ET
C
C     ============================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE FLA.
C
C     ============================================================
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
C
      IF(ARG.GT.1.6D2) ARG=1.6D2
      IF(ARG.LT.-1.6D2) ARG=-1.6D2
      A=DLOG(ARG)
      B=EF-ARG
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=(1.0D0+DEXP(B))
      IF(DENOM.GT.1.0D70) DENOM=1.0D70
      IF(DENOM.LT.-1.0D70) DENOM=-1.0D70
      DENOM=DLOG(DENOM)
      YINT=A-B
      IF(YINT.GT.1.6D2) YINT=1.6D2
      IF(YINT.LT.-1.6D2) YINT=-1.6D2
      YINT=DEXP(YINT)
C
C
      RETURN
      END
```

```
C
C     ================================================================
C
C     FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
C                      METALLIC CONDUCTOR
C
C     USAGE:   REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.
C
C     ================================================================
C
      FUNCTION EFERMI(EF,DUMMY)
      DIMENSION DUMMY(10)
      EXTERNAL XINT
C
C     -----INTEGRATE FROM 0 TO INF-----
C
      EF0=DUMMY(1)
      DUMMY(2)=EF
      SUM=0.0D0
      XX=EF-1.2D1
      IF(XX.GT.0.0D0) SUM=2.0D0*(XX**(3.0D0/2.0D0))/3.0D0
      XUBND=0.0D0
      IF(XX.GT.0.0D0) XUBND=XX
   10 CONTINUE
      XLBND=XUBND
      XUBND=XUBND+1.0D1
      XX=XUBND-EF
      IF(XX.GT.1.0D2) GOTO 30
      CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
      SUM=SUM+RES
      GOTO 10
C
   30 CONTINUE
      EFERMI=1.0D0-3.0D0*EF0**(-3.0D0/2.0D0)*SUM/2.0D0
C
C
```

```
      RETURN
      END
```

APPENDIX 1-H

Program for Calculating Many Equilibrium Characteristics of Silicon Throughout a Specified Range of Temperature

```
C
C     ====================================================
C
C     MAIN PROGRAM FOR CALCULATING THE EQULIBRIUM CHARACTERISTICS
C     OF P-TYPE SILICON VS. TEMPERATURE
C
C               THE CHARACTERISTICS CALCULATED ARE:
C                   XION=IONIZED ACCEPTOR DENSITY
C                   VDIFF=DIFFUSION POTENTIAL FOR A GIVEN BARRIER
C                   EIF=FERMI ENERGY DISTANCE FROM INTRINSIC FERMI
C                       ENERGY,EI---IN EV
C                   EIV=INTRINSIC FERMI ENERGY,EF, DISTANCE FROM
C                       THE VALENCE BAND EDGE, EC---IN EV
C                   HEQI=EQULIBRIUM HOLE DENSITY IN SILICON
C                   ENSUBI= INTRINSIC HOLE/ELECTRON DENSITY AT
C                           SPECIFIED TEMP.
C                   EGAP=ENERGY GAP OF FORBIDDEN BAND
C
C
C
C     USEAGE: REQUIRES SUBROUTINE XTEMPR AND FUNCTION EQU
C
C             BRRIER=ASSUMED BARRIER AT SI/METAL INTERFACE
C             TEMP=STARTING STEP FOR TEMPERATURE
C             TDLT=STEP SIZE FOR TEMP
C             IMAX=NUMBER OF TEMP STEPS
C             ACCPTR=STARTING STEP FOR ACCEPTOR DENSITY
C             ADLT=STEP SIZE FOR ACCPTR
C             JMAX=NUMBER OF ACCPTR STEPS
C
C             LUOUT=CHANNEL FOR OUTPUT
C
C
C     ====================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.
C
C     ====================================================
C
C     -----INITIALIZE MISC CONSTANTS-----
```

```
C
      ACCPTR=1.ØD11
      ADLT=1.ØD1
      JMAX=7
      TEMP=7.ØD1
      TDLT=1.ØD1
      IMAX=24
      BRRIER=Ø.27DØ
      BOLTZ=.Ø2585DØ
C
      LUOUT=1Ø
C
C     -----TOP OF ACCPTR STEPPING LOOP-----
C
C
      DO 5Ø J=1,JMAX
      ACCPTR=ACCPTR*1.ØD1
      WRITE(LUOUT,1111) ACCPTR
 1111 FORMAT(1X,1PD1Ø.3)
C
C     -----TOP OF TEMP STEPPING LOOP-----
C
      T=TEMP
      DO 1Ø I=1,IMAX
C
      CALL XTEMPR(XION,ENSUBI,VDIFF,EIF,EIV,T,HOLES,EGAP,BOLTZ,ACCPTR,
     &BRRIER,LUOUT)
      WRITE(LUOUT,1ØØØ) T,XION,HOLES,ENSUBI,EGAP,EIF,EIV,VDIFF
 1ØØØ FORMAT(1X,'T=',F6.1,3X,'XION=',1PD1Ø.3,3X,'HOLES=',1PD1Ø.3,3X,
     &'NI=',1PD1Ø.3,3X,'EG=',1PD9.2,3X,'EIF=',1PD9.2,3X,'EIV=',
     &1PD9.2,3X,'VDIFF=',1PD9.2)
C
      T=T+TDLT
   1Ø CONTINUE
C
C
   5Ø CONTINUE
      END
```

```
C
C     ================================================================
C
C     SUBROUTINE XTEMPR:IS USED TO CALCULATE MANY TEMP DEPENDENT
C                       PROPERTIES OF SILICON, IN ADDITION TO THE
C                       DIFF POTENTIAL OF A PT-SI BARRIER
C
C                       XION=IONIZED BORON ATOMS (CM**-3)
C                       ENSUBI=NI (CM**-3)
C                       VDIFF=DIFF POTENTIAL (VOLTS)
C                       EIF=EI-EF IN EV
C                       EIV=EI-EV IN EV
C                       TEMP=TEMPERATURE  DEG.K
C                       HOLES=HOLE DENSITY (CM**-3)
C                       EGAP=ENERGY GAP IN EV
C                       ACCPTR=ACCPTR DENSITY (CM**-3)
C                       BARRER=ENERGY BARRIER (EV) FOR VDIFF CALC
C                       BOLTZ=BOLTZMANN CONSTANT AT 300 DEG. K
C
C                       LUOUT=OUTPUT CHANNEL
C
C
C     USEAGE: REQUIRES SUBROUTINE ROOT AND FUNCTION EQU
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC.. GAINESVILLE FLA.
C
C     ================================================================
C
      SUBROUTINE XTEMPR(XION,ENSUBI,VDIFF,EIF,EIV,TEMP,HOLES,EGAP,BOLTZ.
     $ACCPTR,BRRIER,LUOUT)
      DIMENSION DUMMY (11)
      EXTERNAL EQU
C
C
      T=TEMP/3.D2
      EGAP=1.165-7.242D-3*T-3.664D-2*T*T
      EIV=EGAP/2.D0-1.396D-2*T
      ENSUBI=3.925D19*T*DSQRT(T)*DEXP(-EGAP/(2.0D0*BOLTZ*T))
```

```
C
C
      DUMMY(1)=EGAP
      DUMMY(2)=EIV
      DUMMY(3)=ENSUBI
      DUMMY(4)=T
      DUMMY(5)=BOLTZ
      DUMMY(6)=BRRIER
      DUMMY(7)=ACCPTR
C
      EIF=EIV
      EIFMX=-EIV
      DLTEI=-EIV/2.ØD1
C
      CALL ROOT(EQU,EIF,EIFMX,DLTEI,1.ØD-6,Ø,IER,DUMMY)
C
      IF(IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND IN XTEMPR'
C
      XION=DUMMY(8)
      EAF=DUMMY(9)
      EFV=DUMMY(1Ø)
      HOLES=DUMMY(11)
C
      VDIFF=BRRIER-EFV
C
      RETURN
      END
```

```
      FUNCTION EQU(EIF,DUMMY)
C
      DIMENSION DUMMY(11)
C
      EGAP=DUMMY(1)
      EIV=DUMMY(2)
      ENSUBI=DUMMY(3)
      T=DUMMY(4)
      BOLTZ=DUMMY(5)
      BRRIER=DUMMY(6)
      ACCPTR=DUMMY(7)
C
      EFV=EIV-EIF
      EAF=4.38D-2-3.037D-8*ACCPTR**(1.0/3.0)-EFV
      XION=1.0D0/(1.0+(4.0+2.0/DEXP(4.4D-2/(BOLTZ*T)))*DEXP(EAF/(BOLTZ*T)))
      XION=XION*ACCPTR
C
      HOLES=ENSUBI*DEXP(EIF/(BOLTZ*T))
      EQU=(HOLES-XION)/ACCPTR
C
      DUMMY(8)=XION
      DUMMY(9)=EAF
      DUMMY(10)=EFV
      DUMMY(11)=HOLES
C
      RETURN
      END
```

APPENDIX 1-I

Program for Numerically Solving Poisson's Equation for a One-Dimensional Schottky Barrier

```
C
C     ================================================================
C
C     MAIN ADMINISTRATIVE PROGRAM FOR CALCULATING THE REVERSE CURRENT
C     OF A SCHOTTKY BARRIER ON P-TYPE SILICON.
C
C     ================================================================
C
C     ORIGINAL:D.P. KENNEDY & ASSOC., GAINESVILLE FLA.
C
C     ================================================================
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
C     -----INITIALIZE MISC CONSTANTS-----
C
      ACCPTR=1.0D15
      TEMP=7.7D1
      VAPPL0=0.0D0
      VDELT=0.0D0
      NSTEP=1
      BRRIER=2.7D-1
      LUIN=11
      LUIN2=LUIN
      LUOUT=10
```

```
      LUOUT2=LUOUT
C
C     -----CALCULATE EQULIB. CHARACTERISTICS OF SI AT TEMP-----
C
      CALL EQULIB
C
C     -----NORMALIZE ALL PARAMETERS-----
C
      CALL NRMLIZ
C
C     ======================================
C     TOP OV VOLTAGE STEPPING LOOP
C     ======================================
C
      NCOUNT=1
      VAPPL=VAPPL0-VDELT
   20 CONTINUE
      VAPPL=VAPPL+VDELT
C
      CALL GRID
C
      CALL LMATRIX
C
      CALL INITIAL
C
      CALL HOLES
C
      CALL CHARGE
C
      CALL PICARD
C
      NCOUNT=NCOUNT+1
      IF (NCOUNT.GT.NSTEP) GOTO 30
C
C     CALL OUTPUT
C
      GOTO 20
C
   30 CONTINUE
      STOP
C
C
```

```
      END
C
C
C
```

```
      SUBROUTINE EQULIB
C
C     ================================================================
C
C     USING UNNORMALIZED VARIABLES, CALCULATES THE TEMPERATURE-
C     DEPENDENT BAND GAP, THE IONIZED ACCEPTOR DENSITY,AND THE BUILT-IN
C     POTENTIAL BARRIER, ACCOUNTING FOR THE TEMPERATURE DEPENDENCE OF
C     THE INTRINSIC DENSITY AND OF THE FERMI LEVEL.
C
C     ================================================================
C
C     ORIGINAL:D.P. KENNEDY &ASSOC., GAINESVILLE FLA.
C
C     ================================================================
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BARRER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XIQN,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
      NDOPE=0.0D0
      T=TEMP/3.D2
      BOLTZ=0.02585*T
      EGAP=1.165-7.242D-3*T-3.664D-2*T*T
      EIV=EGAP/2.D0-1.306D-2*T
      X=EIV
      KEY=1
      GO TO 170
```

```
C
C     -----ADJUST X1&X2 UNTIL Y1&Y2 HAVE OPPOSITE SIGN-----
C
  100 X1=X
      Y1=Y
      DX=-EIV/2.D1
      IF(Y.LT.0.) DX=-DX
      X=X1+DX
      KEY=2
      GO TO 170
  110 X2=X
      Y2=Y
      IF(Y1*Y2.LE.0.) GO TO 140
      X1=X2
      Y1=Y2
      X=X2+DX
      GO TO 170
  140 KEY=3
C
C     -----METHOD OF SECANTS-----
C
  150 IF(DABS(Y).LT.1.D-3) GO TO 180
      DEN=Y2-Y1
      X=(X1*Y2-X2*Y1)/DEN
      GO TO 170
  160 X1=X2
      Y1=Y2
      X2=X
      Y2=Y
      GO TO 150
C
C     -----SUBROUTINE FOR EVALUATING Y-----
C
  170 EIF=X
      EFV=EIV-EIF
      EAF=4.38D-2-3.037D-8*ACCPTR**(1.0/3.0)-EFV
      XION=ACCPTR/(1.0+(4.0+1.0/DEXP(4.4D-2/BOLTZ))*DEXP(EAF/BOLTZ))
      ENSUBI=3.925E19*T*DSQRT(T)*DEXP(-EGAP/(2.*BOLTZ))
      HEQUI=ENSUBI*DEXP(EIF/BOLTZ)
      Y=(HEQUI-XION)/ACCPTR
      GO TO(100,110,160),KEY
C
```

```
      VDIFF=BARRER-EFV
      WRITE(LUOUT2,1000)TEMP,EGAP,EIV,EIF,EFV,ENSUBI,XION,VDIFF
 1000 FORMAT(2X,//,3X,'TEMP',5X,'EGAP',7X,'EIV',7X,'EIF',7X,'EFV',
     36X,'ENSUBI',4X,'XION',4X,'VDIFF',//,1X,1P8E10.2,//)
      RETURN
      END
```

```
      SUBROUTINE NRMLIZ
C
C     ------------------------------------------------------
C     SUBROUTINE NRMLIZE IS USED TO NORMALIZE FREQUENTLY USED
C     .                  PARAMETERS FOR THE ANALYSIS OF A
C     .                  SCHOTTKY BARRIER ON P-TYPE SILICON
C     ------------------------------------------------------
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
      DNSNRM=XION
      PSINRM=BOLTZ
      DEBYE=DSQRT(11.7*8.85D-14*BOLTZ/(1.6D-19*XION))
      TEMPNRM=3.0D2
C
C
      VAPPL0=VAPPL0/PSINRM
      VDLT=VDLT/PSINRM
      VDIFF=VDIFF/PSINRM
      XLNGTH=XLNGTH/DEBYE
      XJNCTN=XJNCTN/DEBYE
      XION=XION/DNSNRM
C
      RETURN
      END
```

```
 10 / 21 / 1981              7 : 6 : 18                    GRID.GV

      SUBROUTINE GRID
C
C     ================================================================
C
C     SUBROUTING GRID SETS UP LATTICE PARAMETERS FOR THE FINITE DIFF.
C     ARRAYS
C
C     ================================================================
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
      WRITE(LUOUT2)'SUBROUTINE GRID'
C
C     -----CALC LENGTH OF SI REGION-----
C
      WD=DSQRT(2.0D0*(VAPPL+VDIFF)/XION)
      WD=1.5D0*WD
C
      XJNCTN=WD*1.0D-1
      XLNGTH=WD*1.1D0
C
C     -----SET GRID SPACING-----
C
      JMAX=WD
      IF(JMAX.LT.100) JMAX=200
```

```
      JUNCTN=JMAX/10
      XDELT1=1.0D0
      XDELT2=1.0D0
C
C     -----PTSI REGION-----
C
      SUM=1.0D0
      JMAXX=JUNCTN-2
      DO 10 J=1,JMAXX
      SUM=SUM+XDELT1**J
   10 CONTINUE
C
      XDLT(1)=XJNCTN/SUM
      JMAXX=JUNCTN-1
      DO 20 I=1,JMAXX
      XDLT(I+1)=XDLT(I)*XDELT1
   20 CONTINUE
C
C
      XPOS(1)=0.0D0
C
      DO 30 J=2,JUNCTN
      XPOS(J)=XPOS(J-1)+XDLT(J-1)
   30 CONTINUE
C
C     ----- SILICON REGION -----
C
      SUM=1.0D0
      JMAXX=JMAX-JUNCTN-1
      DO 40 J=1,JMAXX
      SUM=SUM+XDELT2**J
   40 CONTINUE
C
      XDLT(JMAX-1)=WD/SUM
      KMAXX=JMAX-JUNCTN
      DO 50 K=2,KMAXX
      J=JMAX-K
      XDLT(J)=XDLT(J+1)*XDELT2
   50 CONTINUE
C
C
      JMINN=JUNCTN+1
```

```
      DO 60 J=JMINN,JMAX
      XPOS(J)=XPOS(J-1)+XDLT(J-1)
   60 CONTINUE
C
      RETURN
      END
```

```
C
C     ================================================================
C
C     SUBROUTINE LMATRIX SETS UP THE FINITE-DIFFERENCE MATRIX FOR SOLVING
C     .                  POISSN'S EQUATION. THEREAFTER THIS MATRIX IS
C     .                  SUBJECTED TO A CHOLOSKY DECOMPOSITION YIELDING
C     .                  A LOWER DIAGONAL L MATRIX.
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.
C
C     ================================================================
      SUBROUTINE LMATRIX
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPLØ,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
C     ----- SET UP MATRIX FOR POISSNS EQUATION -----
C
      A(1,1)=0.0
      A(1,2)=(XDLT(1)+XDLT(2))/(XDLT(1)+XDLT(2))
      K=0.0D0
C
      JMAXX=JMAX-2
      DO 1 J=2,JMAXX
```

```
      A(J,1)=-1.0D0/XDLT(J)
      A(J,2)=(XDLT(J)+XDLT(J+1))/(XDLT(J)*XDLT(J+1))
    1 CONTINUE
C
C
C
      XD1=1.0D0
      ID2=0
C
      N=JMAX-2
      M=1
C
      DO 70 I=1,N
      IP=M-I+1
      IF (I.GT.M) IP=0
      IR=I-M+IP
C
      DO 60 J=IP,M
      IX=J-1
      IQ=M-J+IP
      JJ=J+1
      Y=A(I,JJ)
      DO 10 K=IP,IX
      KK=K+1
      IIQ=IQ+1
      Y=Y-XL(I,KK)*XL(IR,IIQ)
      IQ=IQ+1
   10 CONTINUE
C
      IF (J.NE.M) GOTO 50
C
      XD1=XD1*Y
C
      IF (Y.NE.0.0D0) GOTO 20
      ID2=0
      GOTO 9998
C
   20 CONTINUE
      IF (DABS(XD1).LT.1.0D0) GOTO 30
      XD1=XD1*0.0625
      ID2=ID2+4
      GOTO 20
```

```
C
   30 CONTINUE
      IF (DABS(XD1).GE.0.0625) GOTO 40
      XD1=XD1*16.0D0
      ID2=ID2-4
      GOTO 30
C
   40 CONTINUE
C
      IF (Y.LT.0.0D0) GOTO 9999
C
      JJ=J+1
      XL(I,JJ)=1.0D0/DSQRT(Y)
      GOTO 60
C
   50 CONTINUE
      JJ=J+1
      MM=M+1
      XL(I,JJ)=Y*XL(IR,MM)
      IR=IR+1
C
   60 CONTINUE
C
C
      RETURN
C
 9998 CONTINUE
      STOP Y=0
C
 9999 CONTINUE
      STOP Y<0
C
      END
```

```
      SUBROUTINE INITIAL
C
C     ================================================================
C     SUBROUTINE INITIAL IS USED TO INITIALIZE ARRAYS PRIOR TO
C     .                 ENTERING PICARD AND UNDERTAKING AN
C     .                 ITERATIVE SOLUTION FOR THE SCHOTTKY
C     .                 BARRIER PROBLEM
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.
C
C     ================================================================
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /ID/ LUIN,LUIN2,LUOUT,LUOUT2
C
C     ----- CALCULATE DEPLETION LAYER WIDTH -----
C
      WD=DSQRT(2.0D0*(VAPPL+VDIFF)/XION)
C
C     ----- INITIALIZE METAL POTENTIAL --- -
C
C
      DO 10 J=1,JUNCTN
      U(J)=VAPPL+VDIFF
   10 CONTINUE
```

```
C
C
C     ----- INITIALIZE DEPLETION LAYER POTENTIAL -----
C
      JMINN=JUNCTN+1
      DO 20 J=JMINN,JMAX
      XX=XPOS(J)-XPOS(JUNCTN)
      IF(XX.GE.WD) GOTO 30
   20 CONTINUE
C
C
   30 CONTINUE
C
C     ----- INITIALIZE REMAINING U ARRAY -----
C
      JJ=J
      DO 40 J=JJ,JMAX
      U(J)=0.000
   40 CONTINUE
C
C
      RETURN
C
      END
```

```
      SUBROUTINE HOLES
C
C     ================================================
C     SUBROUTINE HOLES IS USED TO CALCULATE THE HOLE DENSITY
C     .              WITHIN A P-TYPE SHOTTKY BARRIER
C     ================================================
C
      ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.
C
C     ================================================
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
     $,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
C     ----- CALCULATE HOLE DENSITY DISTRIBUTION -----
C
      HDENS(JMAX)=XION
      KMAXX=JMAX-JUNCTN
      DO 10 K=1,KMAXX
      J=JMAX-K
      UDLT=U(J)-U(J+1)
      IF(UDLT.GT.1.0D2) UDLT=1.0D2
      IF(UDLT.LT.-0.0D0) UDLT=0.0D0
      IF(HDENS(J+1).LE.1.0D-30) UDLT=0.0D0
      IF(HDENS(J+1).GT.1.0D30) UDLT=0.0D0
      HDENS(J)=HDENS(J+1)*DEXP(-UDLT)
```

```
C     TYPE J,HDENS(J)
      IF(HDENS(J).LE.1.0D-50) HDENS(J)=1.0D-50
   10 CONTINUE
C
C
      RETURN
C
      END
```

```
      SUBROUTINE CHARGE
C
C     ================================================================
C
C     SUBROUTINE CHARGE: IS USED TO CALCULATE THE ELECTROSTATIC
C     .                  CHARGE DISTRIBUTION THROUGHOUT THE
C     .                  ONE-DIMENSIONAL SCHOTTKY BARRIER.
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA
C
C     ================================================================
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
C     ----- METALLIC REGION -----
C
      Q(1)=(VAPPL+VDIFF)/XDLT(1)
C
      DO 10 J=2,JUNCTN
      Q(J)=0.0D0
   10 CONTINUE
C
C     ----- ZERO EDENS ARRAY -----
```

```
C
      DO 20 J=1,JMAX
      EDENS(J)=0.0D0
   20 CONTINUE
C
C     ----- SILICON REGION -----
C
      SUM=0.0D0
      JMINN=JUNCTN+1
      JMAXX=JMAX-2
      DO 30 J=JMINN,JMAXX
      QQ=-(XION-HDENS(J)+EDENS(J))
      Q1=-(XION-HDENS(J+1)+EDENS(J+1))
      SUM=SUM+((Q1+QQ)/2.0D0)*XDLT(J)
      Q(J)=QQ*(XDLT(J-1)+XDLT(J))/2.0D0
   30 CONTINUE
      Q(JMAX-2)=-(VAPPL+VDIFF)/XDLT(JMAX-1)
      Q(JUNCTN)=-SUM*(XDLT(JUNCTN-1)+XDLT(JUNCTN))/2.0D0
      Q(JUNCTN)=Q(JUNCTN)*1.07D0
C
C
      RETURN
      END
```

```
      SUBROUTINE PICARD
C
C     ================================================
C     SUBROUTINE PICARD: IS THE ADMINISTRATION PROGRAM FOR A
C     .                  PICARD ITERATION BETWEEN POISSON'S
C     .                  EQUATION AND THE HOLE DISTRIBUTION.
C     ================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.
C
C     ================================================
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTN,VDIFF,VAPPL0,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
      I=0
      N=1
   10 CONTINUE
C
      CALL POISSN
C
C     -----CALC MAX UDELT-----
C
      JJ=0
      UDELT=0.000
      JMAXX=JMAX-1
```

```
      DO 20 J=2,JMAXX
      R=UNEW(J)-U(J)
      IF(DABS(R).LT.DABS(UDELT)) GOTO 20
      JJ=J
      UDELT=R
   20 CONTINUE
C
      P=UDELT*PSINRM
C
      IF(DABS(P).LE.1.0D-4) GOTO 40
C
C     -----UNDER RELAX POTENTIAL-----
C
      URELAX=0.1500
      JMAXX=JMAX-1
      DO 30 J=2,JMAXX
      U(J)=U(J)+URELAX*(UNEW(J)-U(J))
   30 CONTINUE
C
C
      CALL RESID(RESMX)
C
      CALL HOLES
      CALL CHARGE
      N=N+1
      I=I+1
      GOTO 10
C
   40 CONTINUE
C
      RETURN
      END
```

```
C     ================================================================
C
C     SUBROUTINE POISSN: IS USED TO SOLVE POISSON'S EQUATION FOR
C                        A ONE DIMENTIONAL SCHOTTKY BARRIER. THIS
C                        CALCULATION IS BASED UPON THE SECOND STEP
C                        OF THE CHOLOSKY TECHNIQUE FOR THE SOLUTION
C                        OF THE MATRIX EQUATION.
C
C     ================================================================
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.
C
C     ================================================================
C
      SUBROUTINE POISSN
C
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPLØ,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
C     WRITE(LUOUT2)'SUBROUTINE POISSN'
C
      N=JMAX-2
      M=1
      IS=M-1
C
      DO 20 I=1,N
```

```
      IP=0
      IF (I.LE.*` IP=M-I+1
      IQ=I
      Y=Q(I)
C
      KMAX=IS+*`-IP
      DO 10 KK=`,KMAX
      K=IS+1-KK
      IQ=IQ-1
      JK=K+1
      Y=Y-XL(I,JK)*UNEW(IQ+1)
   10 CONTINUE
C
      MM=M+1
      UNEW(I+1`=Y*XL(I,MM)
C
   20 CONTINUE
      DO 40 IX=`,N
      I=N+1-IX
      IP=0
      IF (N-I.LE.M) IP=M-N+I
      Y=UNEW(I+`)
      IQ=I
C
      KMAX=IS+*`-IP
      DO 30 KK=`,KMAX
      K=IS+1-K`
      IQ=IQ+1
      JK=K+1
      Y=Y-XL(IG,JK)*UNEW(IQ+1)
   30 CONTINUE
C
      MM=M+1
      UNEW(I+` =Y*XL(I,MM)
C
   40 CONTINUE
C
      RETURN
      END
C
C
```

```
      SUBROUTINE RESID (RESMX)
C
C     ------------------------------------------------------
C     SUBROUTINE RESID: IS USED TO CALCULATE THE RESIDUALS
C     .                 ARISING FROM A CHOLOSKY SOLUTION OF
C     .                 POISSON'S EQUATION. THESE RESIDUALS
C     .                 ARE STORED IN THE Q(J) ARRAY AND THE
C     .                 MAXIMUM RESIDUAL PASSED TO THE CALLING
C     .                 SUBROUTINE.
C     ------------------- ------------------------------
C
C     ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.
C
C     -------------------------- ----------------------
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDLT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ITTL(200)
      COMMON /COM10/ UNEW(200)
C
      COMMON /INTGR/ JMAX,JUNCTN,NSTEP
      COMMON /NRMLZE/ DNSNRM,PSINRM,DEBYE
      COMMON /XREAL/ BRRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
     &,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLNGTH,XJNCTN,BOLTZ
      COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2
C
C
      RESMX=0.0D0
C
C
C     ----- CALCULATE RESIDUAL -----
C
C
C
      R=Q(1)-A(1,2)*UNEW(2)-A(2,1)*UNEW(3)
```

```
      RR=DMAX1(DABS(R),RESMX)
      IF(RR.GT.RESMX) RESMX=RR
C
      JMAXX=JMAX-3
      DO 10 J=2,JMAXX
      R=Q(J)-A(J,1)*UNEW(J)-A(J,2)*UNEW(J+1)-A(J+1,1)*UNEW(J+2)
      RR=DMAX1(DABS(R),RESMX)
      IF(RR.GT.RESMX) RESMX=RR
   10 CONTINUE
C
      R=Q(JMAX-2)-A(JMAX-2,1)*UNEW(JMAX-2)-A(JMAX-2,2)*UNEW(JMAX-1)
      RR=DMAX1(DABS(R),RESMX)
      IF(RR.GT.RESMX) RESMX=RR
C
C
C
C
      RETURN
      END
```

APPENDIX II

Temperature Dependent Properties of Silicon

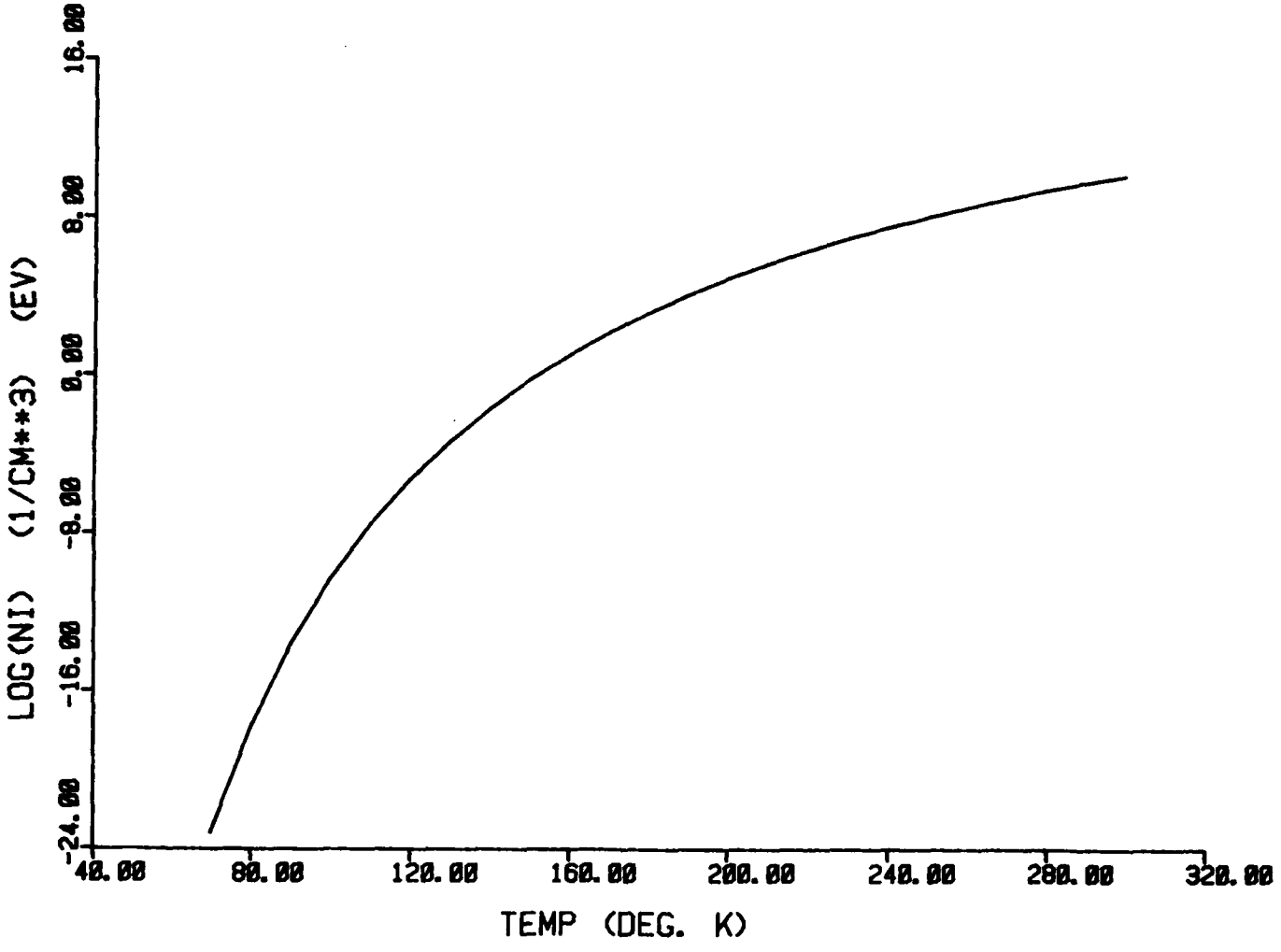


Fig. 29 Intrinsic Carrier Density in Silicon

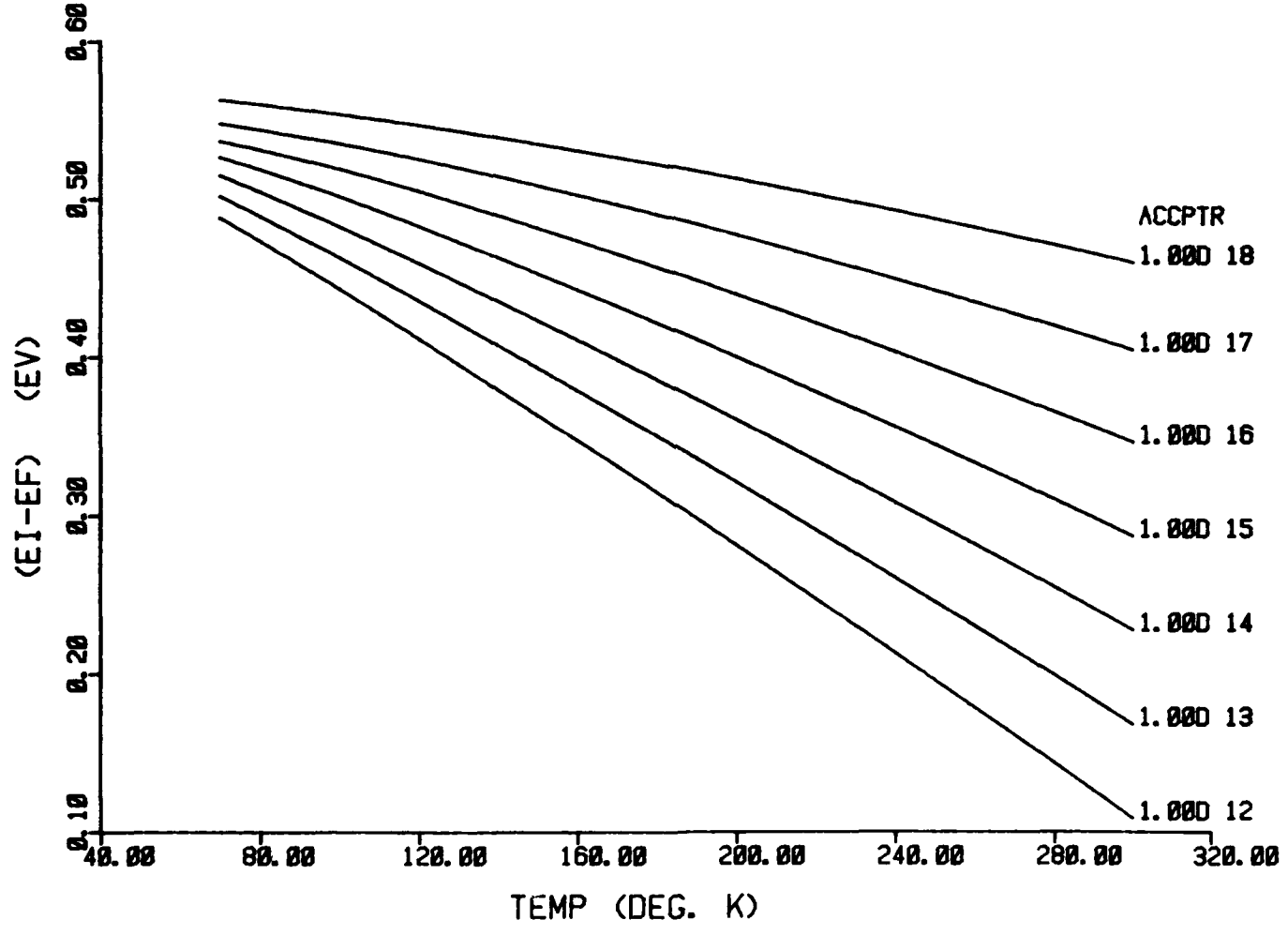


Fig.30 $E_i - E_f$ in Silicon, Where E_i is the Intrinsic Fermi-Level and E_f is the Fermi-Level at the Specified Temperature

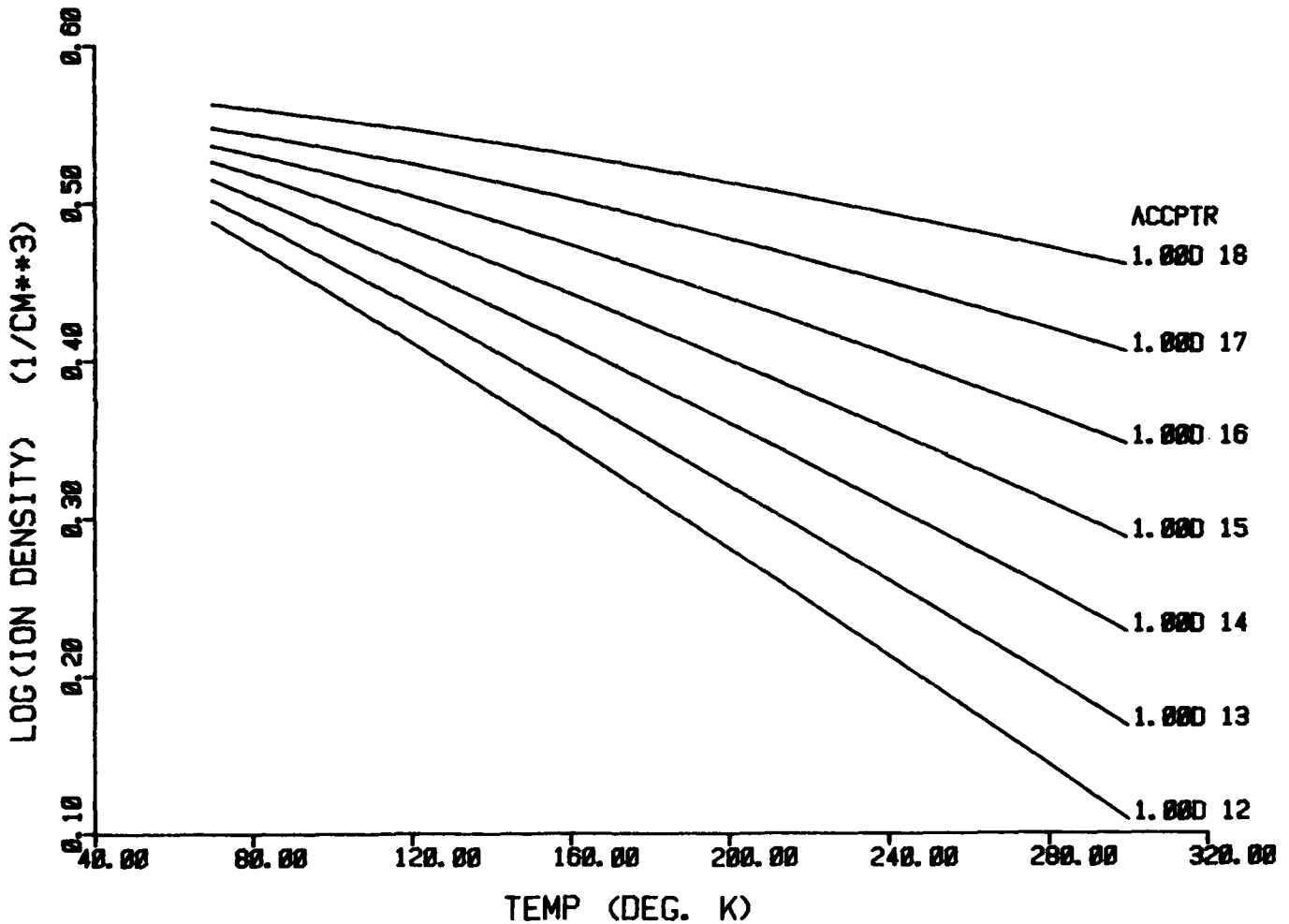


Fig.31 Ionized Impurity Atom (Boron) Density in Silicon

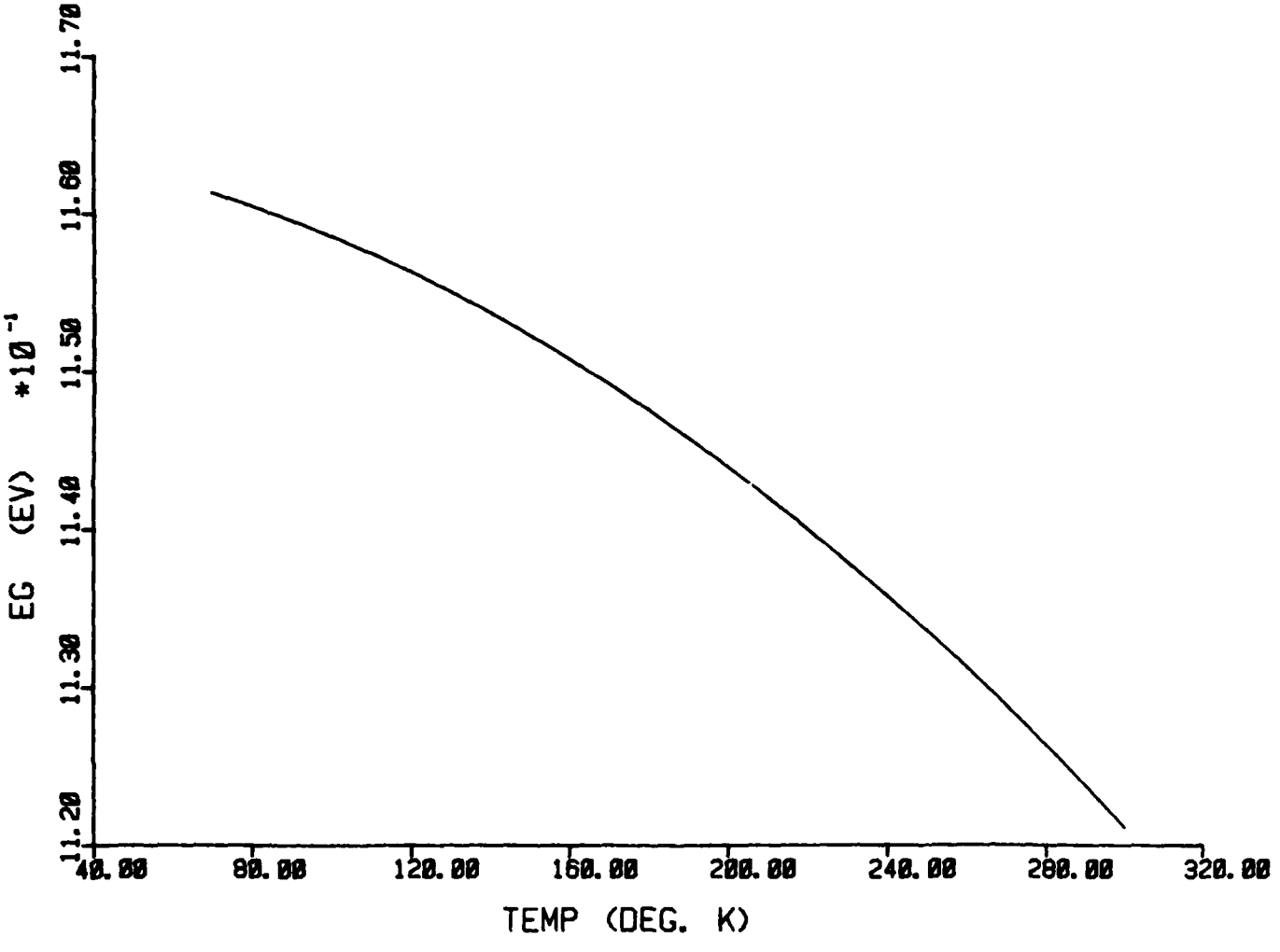


Fig.32 Energy Gap of Silicon

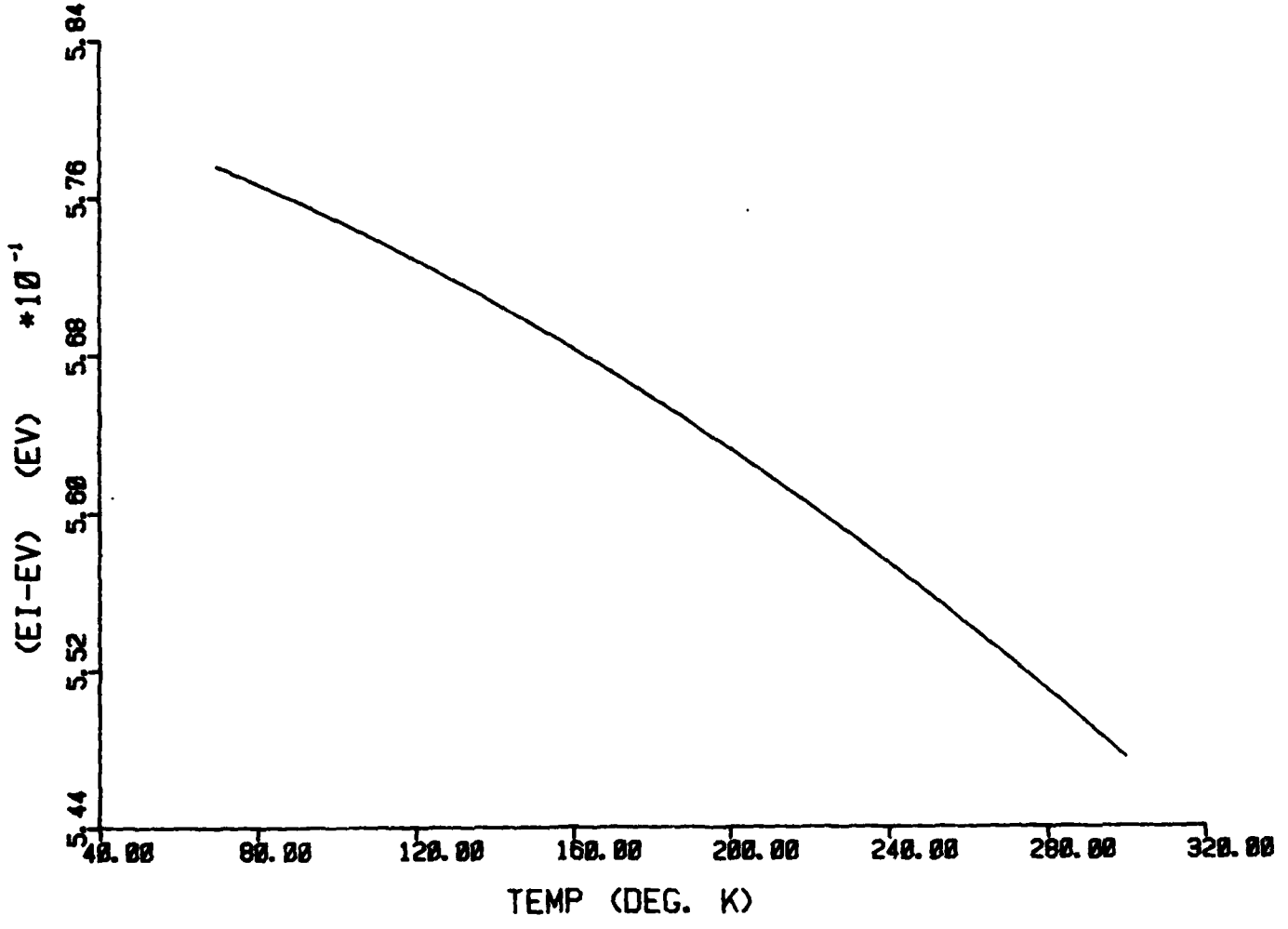


Fig.33 (E_i - E_v) Where in Silicon E_i is the Fermi-Level in Intrinsic Material and E_f is the Fermi-Level at the Specified Temperature

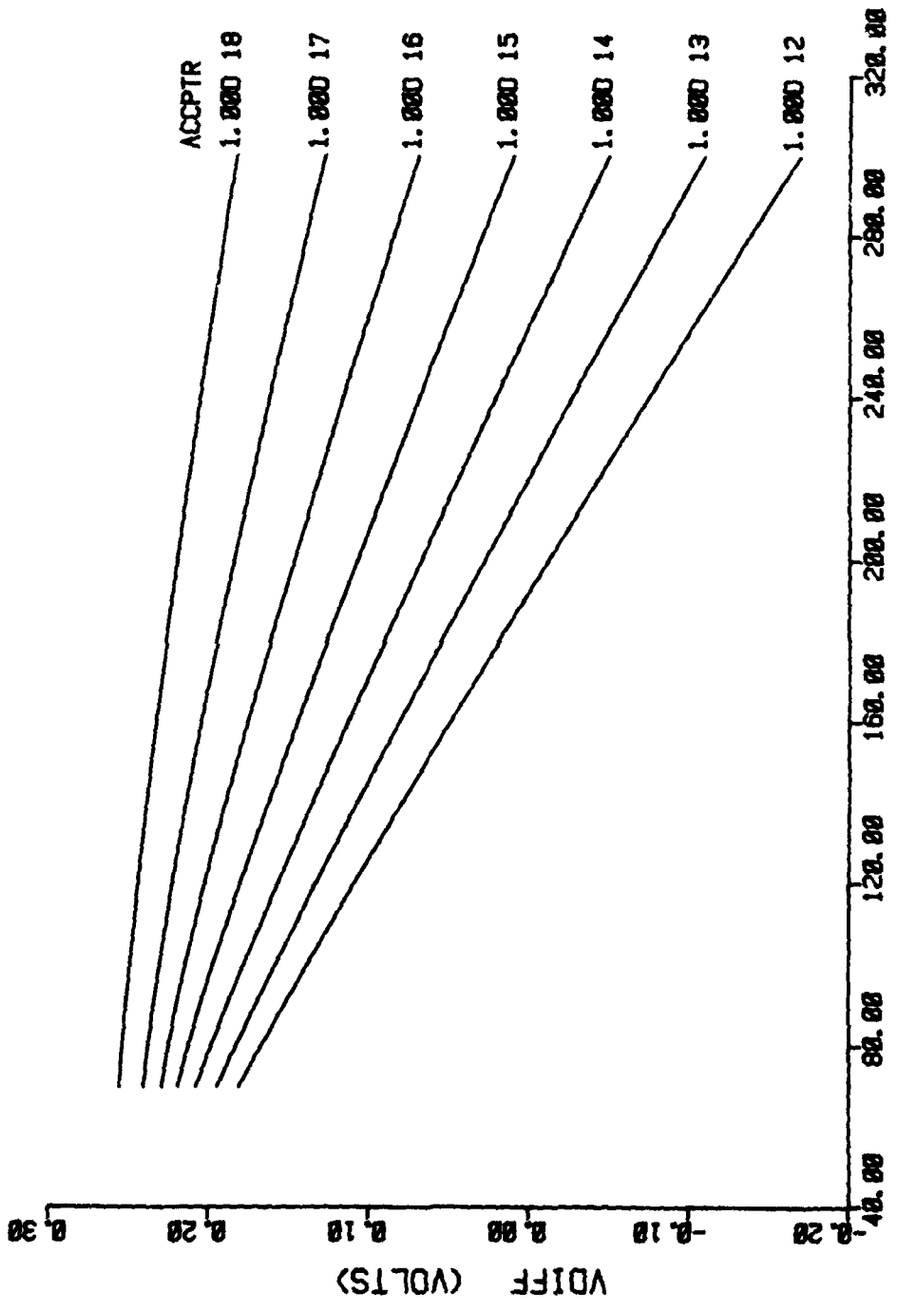


Fig.34 Diffusion Voltage in a Pt-Si Barrier Assuming a Barrier Height of 0.27 ev

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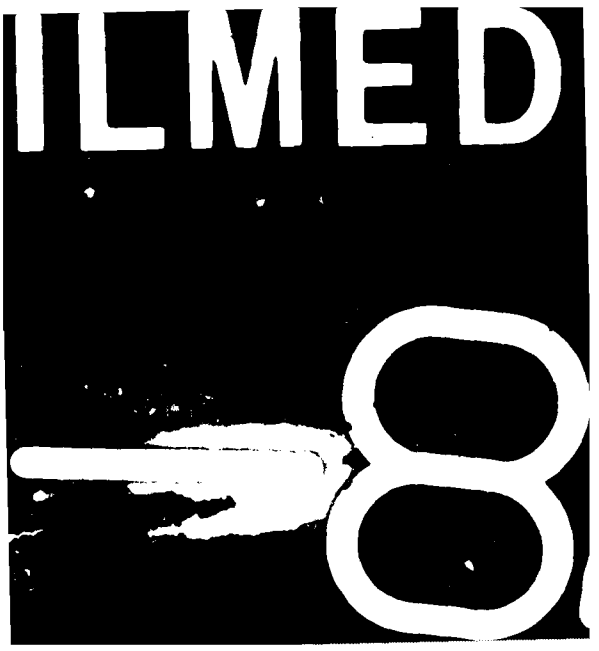
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